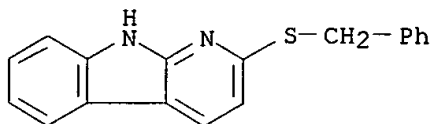


L18 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 26148-35-6 REGISTRY  
CN 9H-Pyrido[2,3-b]indole, 2-(benzylthio)- (8CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C18 H14 N2 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER  
(\*File contains numerically searchable property data)



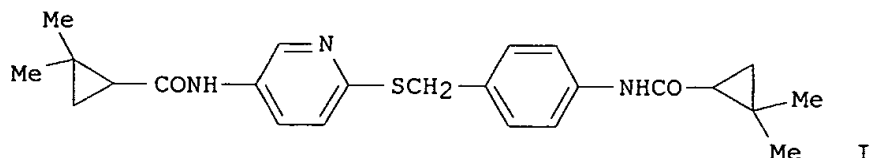
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

OK

AN 2001:31464 CAPLUS  
 DN 134:100762  
 ED Entered STN: 12 Jan 2001  
 TI Preparation of pyridine derivatives and medicinal use thereof  
 IN Iino, Yukio; Fujita, Kohichi; Kodaira, Ariko; Hatanaka, Toshihiro;  
 Takehana, Kenji; Kobayashi, Tsuyoshi; Konishi, Atsushi; Yamamoto, Takashi  
 PA Ajinomoto Co., Inc., Japan  
 SO PCT Int. Appl., 86 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA Japanese  
 IC C07D211-58; C07D213-75; C07D213-76; C07D237-20; C07D237-22; C07D239-42;  
 C07D239-48; C07D277-44; A61K031-44; A61K031-445; A61K031-50; A61K031-505;  
 A61P029-00  
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 1  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002359	A1	20010111	WO 2000-JP4298	20000629
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1193255	A1	20020403	EP 2000-940879	20000629
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000012046	A	20020514	BR 2000-12046	20000629
	TW 519538	B	20030201	TW 2000-89113050	20000630
	US 2002133005	A1	20020919	US 2001-29871	20011231
PRAI	JP 1999-187959	A	19990701		
	JP 2000-71706	A	20000315		
	WO 2000-JP4298	W	20000629		
OS	MARPAT 134:100762				
GI					



AB Heterocyclic compds. represented by the following general formula  
 $R1-CO-N(R2)-A-X-B-N(R3)-Y-(CH_2)_n-R4$  [R1 = (un)substituted or cycloalkenyl;  
 R2, R3 = H, alkyl; R4 = (un)substituted alkyl, alkenyl, cycloalkyl,  
 cycloalkenyl, aryl, or heterocyclyl having .gtoreq.1 heteroatom(s); A =  
 (un)substituted heterocyclic ring; B = (un)substituted arom. or  
 heterocyclic ring; n = 0-6; Y = a bond between atoms, CO, CO<sub>2</sub>, CONR<sub>5</sub>,  
 C(S)NR<sub>5</sub>, SO, SO<sub>2</sub> (wherein R<sub>5</sub> = H, alkyl); X = a bond between atoms, O,  
 OCHR<sub>7</sub>, CHR<sub>8</sub>, O<sub>2</sub>C, CO<sub>2</sub>, OC(S), C(S)O, S, SO, SO<sub>2</sub>, SCHR<sub>9</sub>, CHR<sub>10</sub>S, SC(O),  
 C(O)S, SC(S), C(S)S, SO<sub>2</sub> NR<sub>11</sub>, NR<sub>12</sub>SO<sub>2</sub>, NR<sub>13</sub>, etc.; R<sub>7</sub> - R<sub>10</sub> = H, alkyl;  
 R<sub>11</sub> - R<sub>13</sub> = H, alkyl, acyl] or pharmacol. acceptable salts thereof are

prepd. These compds. have inhibitory effects on AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor, etc. and are usable as drugs such as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics. Thus, 2-mercapto-5-nitropyridine was treated with NaH in DMF and then alkylated by 1-bromomethyl-4-nitrobenzene at room temp. for 1.5 h to give 2-(4-nitrobenzylthio)-5-nitropyridine which was reduced by Zn/AcOH in THF at room temp. for 16 h to 2-(4-aminobenzylthio)-5-aminopyridine and then acylated by 2,2-dimethylcyclopropanecarbonyl chloride in the presence of Et3N in CH2Cl2 at room temp. for 17 h to give 2-(4-(2,2-dimethylcyclopropanecarbonylamino)benzylthio)-5-(2,2-dimethylcyclopropanecarbonylamino)pyridine (I). I in vitro inhibited NF-kappa B activity with IC50 of 0.015 .mu.g/mL in an assay measuring .beta.-galactosidase activity expressed in HUVEC cells and driven by NF-kappa B-binding sequence-fused SV40 T antigen min. promoter.

ST pyridine prepn antiinflammatory; antirheumatic pyridine prepn; **antiviral** immunosuppressant pyridine prepn; cancer metastasis inhibitor pyridine prepn; antiarteriosclerotics pyridine prepn

IT Transcription factors  
 RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
 (AP-1 (activator protein 1); prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Transcription factors  
 RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
 (NF-kappa B (nuclear factor kappa B); prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Cell adhesion  
 (factor, inflammatory; prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Cytokines  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (inflammatory; prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Antitumor agents  
 (metastasis; prepn. of pyridine derivs. as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics)

IT Anti-inflammatory agents  
 Antiarteriosclerotics  
 Antirheumatic agents  
**Antiviral** agents  
 Immunosuppressants  
 (prepn. of pyridine derivs. as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics)

IT 318967-19-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 318967-14-5P 318967-15-6P 318967-16-7P 318967-17-8P 318967-18-9P  
 318967-20-3P 318967-21-4P 318967-22-5P 318967-23-6P 318967-24-7P  
 318967-25-8P 318967-26-9P 318967-27-0P 318967-28-1P  
 318967-29-2P 318967-30-5P 318967-31-6P 318967-32-7P 318967-33-8P  
 318967-34-9P 318967-35-0P 318967-36-1P 318967-37-2P 318967-38-3P  
 318967-39-4P 318967-40-7P 318967-41-8P 318967-42-9P 318967-43-0P  
 318967-44-1P 318967-45-2P 318967-46-3P 318967-47-4P 318967-48-5P  
 318967-49-6P 318967-50-9P 318967-51-0P 318967-52-1P 318967-53-2P  
 318967-54-3P 318967-55-4P 318967-56-5P 318967-57-6P 318967-58-7P  
 318967-59-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 81669-70-7, Metalloprotease

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 88-75-5, 2-Nitrophenol 98-09-9, Benzenesulfonyl chloride 98-88-4, Benzoyl chloride 100-02-7, 4-Nitrophenol, reactions 100-11-8, 4-Nitrobenzyl bromide 103-63-9, 2-Bromoethylbenzene 103-71-9, Phenyl isocyanate, reactions 103-72-0, Phenyl isothiocyanate 103-80-0, Phenylacetyl chloride 104-03-0, 4-Nitrophenylacetic acid 108-24-7, Acetic anhydride 122-04-3, 4-Nitrobenzoyl chloride 123-30-8, 4-Hydroxyaniline 554-84-7, 3-Nitrophenol 636-98-6, 1-Iodo-4-nitrobenzene 637-59-2, 3-Phenylpropyl bromide 661-69-8, Hexamethylditin 932-67-2, 3-Cyclohexanecarbonyl chloride 1821-12-1, 4-Phenylbutanoic acid 1849-36-1, 4-Nitrobenzenethiol 2127-09-5, 2-Mercapto-5-nitropyridine 2581-34-2, 3-Methyl-4-nitrophenol 2719-27-9, Cyclohexanecarbonyl chloride 3073-77-6, 2-Amino-5-nitropyrimidine 3958-57-4, 3-Nitrobenzyl bromide 3958-60-9, 2-Nitrobenzyl bromide 4487-59-6, 2-Bromo-5-nitropyridine 4548-45-2, 2-Chloro-5-nitropyridine 4693-91-8, 4-Methoxyphenylacetyl chloride 5339-26-4, 2-(4-Nitrophenyl)ethyl bromide 5365-15-1, 2,2-Dichlorocyclopropanecarbonyl chloride 5418-51-9, 2-Hydroxy-5-nitropyridine 5469-69-2, 3-Amino-6-chloropyridazine 7169-97-3, 2-Acetamido-5-bromopyridine 10313-60-7, 3,4-Dimethoxyphenylacetyl chloride 14221-01-3, Tetrakis(triphenylphosphine)palladium 23056-33-9, 2-Chloro-4-methyl-5-nitropyridine 24424-99-5, Di-tert-butyl dicarbonate 25026-34-0, 4-Chlorophenylacetyl chloride 33332-29-5 39053-78-6, 3,4,5-Trimethoxyphenylacetyl chloride 50541-93-0, 4-Amino-1-benzylpiperidine 50675-57-5, 2,2-Dimethylcyclopropanecarbonyl chloride 54840-15-2, 4-(tert-Butoxycarbonylamino)phenol 55972-71-9, p-Phenylenediamine hydrochloride 60733-34-8, 2-Methylcyclopropanecarbonyl chloride 69097-20-7, Tris(trimethylsiloxy)ethylene 89312-77-6 90403-98-8, 2-Methylcyclohexanecarbonyl chloride 103554-20-7 193204-58-9 318967-66-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 4982-09-6P 13534-97-9P, 5-Amino-2-bromopyridine 24253-19-8P  
 29958-19-8P 32605-02-0P 34295-27-7P 99844-01-6P 109899-69-6P  
 116735-74-1P 318967-60-1P 318967-61-2P 318967-62-3P 318967-63-4P

318967-64-5P 318967-65-6P 318967-67-8P 318967-68-9P 318967-69-0P  
318967-70-3P 318967-71-4P 318967-72-5P 318967-73-6P 318967-74-7P  
318967-75-8P 318967-76-9P **318967-77-0P 318967-78-1P**  
318967-79-2P 318967-80-5P 318967-81-6P 318967-82-7P 318967-83-8P  
318967-84-9P 318967-85-0P 319459-36-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B  
activity, inflammatory cytokine prodn., matrix metalloprotease prodn.,  
expression of inflammatory cell adhesion factor)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

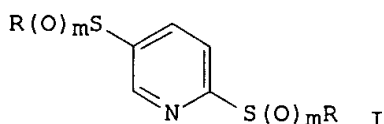
- (1) Ajinomoto Co Inc; WO 200015603 A1 2000
- (2) Boehringer Ingelheim Pharmaceuticals Inc; JP 2000502702 A
- (3) Boehringer Ingelheim Pharmaceuticals Inc; US 6057451 A CAPLUS
- (4) Boehringer Ingelheim Pharmaceuticals Inc; WO 9724343 A1 1997 CAPLUS
- (5) Smithkline Beecham Corp; JP 2000500464 A
- (6) Smithkline Beecham Corp; JP 2000500464 A
- (7) Smithkline Beecham Corp; EP 866700 A1 CAPLUS
- (8) Smithkline Beecham Corp; EP 866700 A1 CAPLUS
- (9) Smithkline Beecham Corp; WO 9717958 A1 1997 CAPLUS
- (10) Smithkline Beecham Corp; WO 9717958 A1 1997 CAPLUS

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OK

AN 1987:32855 CAPLUS  
 DN 106:32855  
 ED Entered STN: 07 Feb 1987  
 TI 2,5-Bis(alkylsulfonyl)- and 2,5-bis(alkylthio)-substituted-pyridines  
 IN Wood, Steven G.  
 PA Dow Chemical Co., USA  
 SO U.S., 9 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07D211-72  
 ICS C07D211-84  
 NCL 546294000  
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 1  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4616087	A	19861007	US 1982-380642	19820521
PRAI	US 1982-380642		19820521		
OS	CASREACT 106:32855				
GI					



AB The title compds. I (R = C1-7 alkyl, cycloalkyl, Ar(CH<sub>2</sub>)<sub>q</sub>, Ar = (un)substituted Ph, naphthyl; q = 0-3; m = 0-2) useful as **antiviral** agents, were prepd. Thus, to 4-F3CSC6H4OH in THF was added Me3COK and 2,5-bis(methylsulfonyl)pyridine, prepd. in 3 steps from Me 3,6-dichloro-2-pyridinecarboxylate, to give 5-(methylsulfonyl)-2-[4-[(trifluoromethyl)thio]phenoxy]pyridine (II). II at 12.5 .mu.g/mL was active against rhinovirus type 1A.

ST pyridine alkylsulfonyl phenoxy prepn **antiviral**  
 IT Virucides and Virustats  
 (bis(alkylsulfonyl)- and bis(alkylthio)-substituted-pyridines)

IT 533-31-3, 3,4-(Methylenedioxy)phenol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with bis(ethylsulfonyl)pyridine)

IT 106-41-2, 4-Bromophenol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with bis(hexylsulfonyl)pyridine)

IT 461-84-7, 4-(Trifluoromethylthio)phenol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with bis(methylsulfonyl)pyridine)

IT 95-77-2, 3,4-Dichlorophenol 99-93-4, p-Hydroxyacetophenone 1137-42-4, p-Hydroxybenzophenone  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with sulfonylpyridines)

IT 85330-64-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and condensation with (methylenedioxy)phenol)

IT 85330-63-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and condensation with (trifluoromethylthio)phenol)

IT 85330-69-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and condensation with bromophenol)  
IT 85330-66-1P 85330-75-2P 85330-79-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with dichlorophenol)  
IT 85330-72-9P 85330-82-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with hydroxyacetophenone)  
IT **85330-78-5P** 85330-89-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with hydroxybenzophenone)  
IT 85330-61-6P 85330-67-2P 85330-70-7P 85330-73-0P **85330-76-3P**  
85331-32-4P 91164-62-4P 106025-37-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and decarboxylation of)  
IT 85331-31-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and decarboxylation-oxidn. of)  
IT 69212-36-8P 85330-62-7P 85330-65-0P 85330-68-3P 85330-71-8P  
85330-74-1P **85330-77-4P** 85330-80-9P 85330-81-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and oxidn. of)  
IT 98626-97-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)  
IT 85330-84-3P 85330-85-4P 85330-86-5P 85330-87-6P 85330-88-7P  
85330-90-1P 85330-91-2P 85330-92-3P 85330-93-4P 85330-96-7P  
85330-97-8P 85330-98-9P 85330-99-0P 85331-02-8P 85331-03-9P  
85331-04-0P 85331-05-1P 85331-06-2P 85331-07-3P 85331-08-4P  
85331-09-5P 85331-10-8P 85331-11-9P 85331-12-0P 85331-13-1P  
85331-14-2P 85331-15-3P 85331-16-4P 85331-17-5P 85331-18-6P  
85331-25-5P 85331-26-6P 85331-27-7P 85331-28-8P 85345-64-8P  
85368-98-5P 99902-97-3P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of, as virucide)  
IT 74-93-1, reactions 75-33-2 111-31-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(substitution by, of Me dichloropyridinecarboxylate)  
IT 75-08-1 100-53-8, Benzyl mercaptan 108-98-5, Thiophenol, reactions  
1569-69-3, Cyclohexyl mercaptan  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(substitution by, of dichloropyridinecarboxylic acid)  
IT 1702-17-6, 3,6-Dichloro-2-pyridinecarboxylic acid 88912-24-7,  
5,6-Dichloro-2-pyridinecarboxylic acid  
RL: PROC (Process)  
(substitution of, with mercaptans)  
IT 1532-24-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(substitution with alkanethiol and hydrolysis of)

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AN 1996:155490 CAPLUS  
 DN 124:202255  
 ED Entered STN: 19 Mar 1996  
 TI Preparation of sulfur-containing heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents  
 IN Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil, Clara I.  
 PA G. D. Searle and Co., USA  
 SO PCT Int. Appl., 212 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D235-28  
 ICS A61K031-415; C07D401-12; A61K031-44; C07D233-84  
 CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9529897	A1	19951109	WO 1995-US5021	19950501
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9523950	A1	19951129	AU 1995-23950	19950501
	US 5945425	A	19990831	US 1996-737251	19961024
	US 2001047038	A1	20011129	US 2001-885221	20010620
PRAI	US 1994-235619	A2	19940429		
	WO 1995-US5021	W	19950501		
	US 1996-659098	B1	19960604		
	US 1999-377888	B1	19990819		
	US 2000-605560	B1	20000627		
OS	MARPAT 124:202255				
AB	The title compds., which are (H+/K+) ATPase inhibitors, useful for the treatment of viral infections, are prep'd. and formulations contg. them are claimed. Thus, 2-[(1H-benzimidazol-2-yl)sulfinylmethyl]-N,N-dimethylbenzenamine, m.p. 107-109.degree., was prep'd. and demonstrated a (H+/K+) ATPase IC50 of 0.7 .mu.M.				
ST	benzimidazolylsulfinylmethylmethylbenzenamine prepn ATPase inhibitor; <b>antiviral</b> agent prepn benzimidazolylsulfinylmethylmethylbenzenamine; benzimidazolyl sulfinylmethylmethylbenzenamine				
IT	Ulcer inhibitors Virucides and Virustats (heterocyclic (H+/K+) ATPase inhibitors)				
IT	9000-83-3, ATPase RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (potassium-hydrogen-activated; prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as <b>antiviral</b> agents)				
IT	55546-06-0P	56713-45-2P	57235-18-4P	60524-97-2P	71670-48-9P
	73590-36-0P	73590-58-6P	73590-61-1P	81527-04-0P	81864-40-6P
	81864-65-5P	94452-40-1P	96733-60-7P	97288-52-3P	97963-93-4P
	97966-85-3P	98412-35-2P	98412-41-0P	99153-80-7P	99153-89-6P
	99499-40-8P	100924-68-3P	101387-98-8P	102127-07-1P	102127-11-7P
	102625-70-7P	102625-79-6P	103014-24-0P	103577-45-3P	103922-27-6P
	103971-24-0P	104340-33-2P	104340-34-3P	104340-35-4P	104340-37-6P
	104340-38-7P	104340-41-2P	104340-86-5P	104524-67-6P	104524-68-7P
	104658-07-3P	104685-57-6P	104987-90-8P	105389-48-8P	105950-65-0P
	105982-35-2P	106746-58-1P	106746-60-5P	106746-61-6P	106746-63-8P



106746-65-0P	106746-66-1P	106746-68-3P	106746-69-4P	106746-76-3P
106746-77-4P	106746-78-5P	106746-79-6P	106746-80-9P	106746-84-3P
106746-86-5P	106746-88-7P	106746-90-1P	106746-93-4P	106746-94-5P
106746-95-6P	106746-96-7P	106746-97-8P	106746-98-9P	106747-00-6P
106747-01-7P	106747-05-1P	106747-06-2P	106747-07-3P	106747-08-4P
106747-09-5P	106747-10-8P	106747-11-9P	106747-12-0P	106747-13-1P
106747-14-2P	106747-15-3P	106747-16-4P	106747-17-5P	106747-18-6P
106747-19-7P	106747-20-0P	106747-21-1P	106747-22-2P	106747-23-3P
106747-24-4P	106747-25-5P	106747-26-6P	106747-27-7P	106747-28-8P
106747-29-9P	106747-30-2P	106747-31-3P	106747-32-4P	106747-33-5P
106747-34-6P	106747-35-7P	106747-36-8P	106747-38-0P	106747-39-1P
106747-40-4P	106747-41-5P	106747-42-6P	106747-43-7P	106747-44-8P
106747-45-9P	106747-47-1P	106747-48-2P	106771-58-8P	106785-95-9P
106785-96-0P	106850-06-0P	107512-17-4P	108026-58-0P	108499-76-9P
108542-66-1P	108662-50-6P	109827-59-0P	110405-59-9P	110754-85-3P
111371-25-6P	111371-35-8P	111476-81-4P	111476-82-5P	111476-83-6P
111476-84-7P	111476-85-8P	111476-86-9P	111476-87-0P	111476-88-1P
111476-89-2P	111476-91-6P	111476-92-7P	111476-93-8P	111476-94-9P
111476-95-0P	111476-96-1P	111476-97-2P	111476-98-3P	111476-99-4P
111477-01-1P	111477-02-2P	111477-03-3P	111477-04-4P	111477-14-6P
111502-75-1P	111604-57-0P	111858-83-4P	112058-72-7P	112058-73-8P
112230-13-4P	112645-53-1P	112705-43-8P	113418-90-9P	113703-12-1P
113703-14-3P	113703-21-2P	113703-22-3P	113703-28-9P	113712-97-3P
113805-04-2P	113855-38-2P	113855-39-3P	113855-40-6P	113855-41-7P
113855-42-8P	113915-02-9P	113942-61-3P	114060-19-4P	114560-55-3P
115046-03-2P	115366-78-4P	115366-80-8P	116091-77-1P	116940-41-1P
117038-05-8P	117046-87-4P	117347-86-1P	117426-11-6P	117934-10-8P
117977-41-0P	118267-21-3P	118267-22-4P	118267-23-5P	118267-24-6P
118267-25-7P	118267-26-8P	118267-27-9P	118267-28-0P	118267-29-1P
118267-30-4P	118267-31-5P	118267-32-6P	118267-33-7P	118267-34-8P
118267-35-9P	118267-36-0P	118267-37-1P	118267-38-2P	118267-39-3P
118267-42-8P	118267-43-9P	118292-92-5P	118292-93-6P	118292-94-7P
118292-95-8P	118292-96-9P	118292-97-0P	118292-98-1P	118292-99-2P
120009-37-2P	120393-57-9P	120699-85-6P	120699-91-4P	120894-65-7P
121050-40-6P	121242-64-6P	121591-86-4P	122223-85-2P	122307-32-8P
122508-81-0P	123215-59-8P	123215-83-8P	123451-58-1P	123823-95-0P
123907-70-0P	123987-02-0P	124736-45-4P	124899-76-9P	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as  
antiviral agents)

IT	125214-42-8P	126026-46-8P	128429-74-3P	128935-96-6P	128936-05-0P
	130049-59-1P	130368-60-4P	130368-62-6P	130368-66-0P	133903-90-9P
	134017-66-6P	134462-81-0P	135430-38-5P	135461-65-3P	135863-25-1P
	137105-02-3P	137247-56-4P	137810-46-9P	139644-93-2P	139767-99-0P
	142062-72-4P	150064-18-9P	150460-06-3P	153284-85-6P	174397-92-3P
	174397-93-4P	174397-94-5P	174397-95-6P	174397-96-7P	174397-97-8P
	174397-98-9P	174397-99-0P	174398-00-6P	174398-01-7P	174398-02-8P
	174398-03-9P	174398-04-0P	<b>174398-05-1P</b>	174398-06-2P	
	174398-07-3P	174398-08-4P	174398-09-5P	174398-10-8P	174398-11-9P
	174398-12-0P	174398-13-1P	174398-14-2P	174398-15-3P	174398-16-4P
	174398-17-5P	174398-18-6P	174398-19-7P	174398-20-0P	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as  
antiviral agents)

IT 144114-21-6, Retropepsin

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as

**antiviral agents)**

IT 85-44-9, Phthalic anhydride 94-09-7, Ethyl 4-aminobenzoate 110-18-9  
140-89-6, Potassium ethylxanthate 400-98-6, 4-(Trifluoromethyl)-2-  
nitroaniline 446-33-3, 3-Fluoro-6-nitrotoluene 455-14-1,  
4-(Trifluoromethyl)aniline 583-39-1, 2-Mercaptobenzimidazole  
1603-41-4, 2-Amino-5-methylpyridine 1635-61-6, 3-Chloro-6-nitroaniline  
1635-84-3, 2,4-Dimethyl-6-nitroaniline 1639-31-2, 3,4,5-Trimethylaniline  
1824-81-3, 2-Amino-6-methylpyridine 2127-03-9, 2,2'-Dipyridyl disulfide  
3171-45-7, 4,5-Dimethyl-1,2-phenylenediamine 3287-79-4,  
2-Mercapto-5,6-dimethylbenzimidazole 5327-33-3, 2-Acetamido-6-  
methylpyridine 5344-90-1, 2-Aminobenzyl alcohol 7595-31-5 25369-78-2  
27231-33-0, 2-Mercapto-4-methylbenzimidazole 27231-36-3 27492-84-8,  
Methyl 4-amino-2-methoxybenzoate 30525-89-4, Paraformaldehyde  
37052-78-1, 2-Mercapto-5-methoxybenzimidazole 39785-37-0,  
4-Methoxy-3,5-dimethylaniline 55489-15-1 71675-52-0,  
2-(Bromomethyl)-4-chloroaniline hydrobromide 71693-08-8,  
2-(Bromomethyl)-5-chloroaniline hydrobromide 74004-74-3 86604-73-1  
88301-76-2 88301-77-3 88301-78-4 88301-79-5 88301-81-9,  
2-(Chloromethyl)aniline hydrochloride 90562-37-1, N-[2-  
(Chloromethyl)phenyl]acetamide 92333-53-4 92643-51-1 92807-01-7  
106746-59-2, 2-(Chloromethyl)-4-methoxyaniline hydrochloride 106746-62-7  
106746-64-9 106746-67-2 106746-71-8 106746-85-4 106746-87-6  
106746-89-8 106746-91-2 106746-92-3 106746-99-0 106771-59-9,  
2-(Chloromethyl)-N,N-dimethylaniline 174397-86-5 174397-87-6  
174397-88-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as

**antiviral agents)**

IT 4093-29-2P, Methyl 4-acetamido-2-methoxybenzoate 25617-34-9P  
27841-33-4P 59338-85-1P, Methyl 4,5-diamino-2-methoxybenzoate  
86847-79-2P 104524-65-4P 106746-72-9P 106746-73-0P 106746-74-1P  
106746-75-2P 106746-81-0P 106746-82-1P 106746-83-2P 106747-02-8P  
106747-03-9P 106747-04-0P 106747-46-0P 106771-57-7P 118267-40-6P  
165685-25-6P 174397-89-8P 174397-90-1P 174397-91-2P 174398-21-1P  
174398-22-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as

**antiviral agents)**

=>

AN 2000:772628 CAPLUS  
 DN 133:321879  
 ED Entered STN: 03 Nov 2000  
 TI Preparation of 5-pyridyl-1,3-azole compounds as antagonists of adenosine  
 A3 receptor, process for producing the same and use thereof  
 IN Ohkawa, Shigenori; Kanzaki, Naoyuki; Miwatashi, Seiji  
 PA Takeda Chemical Industries, Ltd., Japan  
 SO PCT Int. Appl., 152 pp.  
 CODEN: PIXXD2

DT Patent

LA Japanese

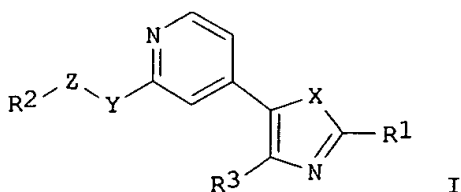
IC ICM C07D417-04

ICS C07D417-14; A61K031-4439; A61P043-00; A61P029-00; A61P031-12;  
 A61P003-10; A61P001-00; A61P009-00; A61P007-00

CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 7

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000064894	A1	20001102	WO 2000-JP2575	20000420
	W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1180518	A1	20020220	EP 2000-917375	20000420
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000009952	A	20020326	BR 2000-9952	20000420
	NZ 515215	A	20030725	NZ 2000-515215	20000420
	AU 765473	B2	20030918	AU 2000-38401	20000420
	JP 2001114779	A2	20010424	JP 2000-126289	20000421
	JP 3333774	B2	20021015		
	JP 2002363179	A2	20021218	JP 2002-164744	20000421
	NO 2001005156	A	20011218	NO 2001-5156	20011022
	ZA 2001008996	A	20030131	ZA 2001-8996	20011031
PRAI	JP 1999-116686	A	19990423		
	JP 1999-224650	A	19990806		
	WO 2000-JP2575	W	20000420		
	JP 2000-126289	A3	20000421		
OS	MARPAT 133:321879				
GI					



$Y = S$   
 $Z = CH_2$   
 $R_2 = \text{aromatic group}$

AB Optionally N-oxidized compds. represented by general formula (I) salts thereof [wherein R1 represents hydrogen, hydrocarbyl, a heterocycle, amino or acyl; R2 represents an arom. group; R3 represents hydrogen, pyridyl or

arom. hydrocarbyl; X represents oxygen or optionally oxidized sulfur; Y represents a bond, oxygen, optionally oxidized sulfur or NR4 (wherein R4 represents hydrogen, hydrocarbyl, or acyl); and Z represents a bond or a divalent chain hydrocarbyl] are prepd. These compds. are usable as preventives or remedies for diseases in assocn. with adenosine A3 receptor because of having excellent adenosine A3 receptor antagonism thereof. Moreover, the compds. I or salts thereof exhibit excellent effects of inhibiting p38 MAP kinase and inhibiting TNF-.alpha. and, therefore, are also usable as preventives or remedies for diseases in assocn. with p38 MAP kinase or TNF-.alpha.. Above diseases include asthma, allergies, brain edema, cerebral vascular disorders, head injuries, inflammation, Addison's disease, autoimmune hemolytic anemia, Crohn's disease, psoriasis, rheumatism, spinal cord injury, multiple sclerosis, Alzheimer's disease, Parkinson's disease, amyotrophic lateral sclerosis, diabetes, arthritis, septemia, ulcerative colitis, chronic pneumonia, silicosis, lung sarcoidosis, pulmonary tuberculosis, cachexia, arteriosclerosis, Creutzfeldt-Jakob disease, virus infection, atopic dermatitis, systemic lupus erythematosus, AIDS encephalopathy, meningitis, angina pectoris, myocardial infarction, ischemic heart failure, hepatitis, transplant, dialysis hypotension, and frequent disseminated intravascular coagulation. Thus, bromination of 2-(2-benzoylamino-4-pyridyl)-1-(4-methoxyphenyl)ethanone with Br in AcOH at room temp. for 1 h followed by cyclocondensation of the bromination product with thiourea in the presence of Et3N in MeCN at 80.degree. for 5 h gave N-[4-[2-amino-4-(4-methoxyphenyl)-1,3-thiazol-5-yl]-2-pyridyl]benzamide (II). II showed IC50 of 0.020 .mu.M against p38 MAP kinase and 0.014 .mu.M for inhibiting the prodn. of TNF-.alpha. in THP-1 cells. II unus  
- AIDS

- ST pyridylazole prepn antagonist adenosine A3 receptor; pyridylthiazole prepn TNF alpha inhibitor; p38 MAP kinase inhibitor pyridylthiazole
- IT Adenosine receptors  
 RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
 (A3; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Brain, disease  
 Prion diseases  
 (Creutzfeldt-Jakob; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Intestine, disease  
 (Crohn's; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Nervous system  
 (amyotrophic lateral sclerosis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Heart, disease  
 (angina pectoris; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Dermatitis  
 (atopic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Brain, disease  
 (cerebrovascular; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Pneumonia  
 (chronic; prepn. of pyridylazole compds. as antagonists of adenosine A3

receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Blood coagulation  
(disseminated intravascular, frequent; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease  
(edema; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease  
(failure, ischemic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Anemia (disease)  
(hemolytic, autoimmune; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease  
(in assocn. with AIDS; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Hypotension  
(in assocn. with dialysis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease  
(infarction; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Head  
Spinal cord  
(injury; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Addison's disease  
Allergy inhibitors  
Alzheimer's disease  
Anti-inflammatory agents  
Antiartherosclerotics  
Antiarthritics  
Antiasthmatics  
Antidiabetic agents  
Antirheumatic agents  
**Antiviral agents**  
Cachexia  
Hepatitis  
Meningitis  
Multiple sclerosis  
Parkinson's disease  
Psoriasis  
Septicemia  
Silicosis  
Transplant and Transplantation  
Tuberculosis  
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Tumor necrosis factors  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Lung, disease  
(sarcoidosis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Lupus erythematosus  
(systemic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Intestine, disease  
(ulcerative colitis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 303162-57-4P 303162-71-2P 303162-72-3P 303162-74-5P 303162-75-6P  
303162-76-7P 303162-77-8P 303162-78-9P 303162-79-0P 303162-80-3P  
303162-85-8P 303162-86-9P 303162-87-0P 303162-88-1P 303162-89-2P  
303162-90-5P 303162-91-6P 303162-92-7P 303162-93-8P 303162-94-9P  
303162-95-0P 303162-96-1P 303163-15-7P 303163-17-9P 303163-18-0P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 303162-58-5P 303162-59-6P 303162-60-9P 303162-61-0P 303162-62-1P  
303162-64-3P 303162-66-5P 303162-67-6P 303162-68-7P 303162-69-8P  
303162-70-1P 303162-73-4P 303162-81-4P 303162-82-5P 303162-83-6P  
303162-84-7P 303162-97-2P 303162-98-3P 303162-99-4P 303163-00-0P  
303163-01-1P 303163-02-2P 303163-03-3P 303163-04-4P 303163-05-5P  
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303163-19-1P 303163-20-4P 303163-21-5P 303163-22-6P 303163-23-7P  
303163-24-8P 303163-25-9P 303163-26-0P 303163-27-1P 303163-28-2P  
303163-29-3P 303163-30-6P 303163-31-7P 303163-32-8P 303163-33-9P  
303163-34-0P 303163-35-1P 303163-36-2P 303163-37-3P 303163-38-4P  
303163-39-5P 303163-40-8P 303163-41-9P 303163-42-0P  
**303163-43-1P** 303163-44-2P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 165245-96-5, p38 MAP kinase  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 62-55-5, Thioacetamide 62-56-6, Thiourea, reactions 64-04-0,  
2-Phenylethylamine 74-88-4, Methyl iodide, reactions 75-36-5, Acetyl  
chloride 75-55-8 98-88-4, Benzoyl chloride 100-07-2,  
4-Methoxybenzoyl chloride 100-46-9, Benzylamine, reactions 100-51-6,  
Benzenemethanol, reactions 100-53-8, Phenylmethanethiol 103-67-3,  
N-Benzyl-N-methylamine 103-80-0, Phenylacetyl chloride 104-86-9,  
4-Chlorobenzylamine 108-98-5, Thiophenol, reactions 109-74-0,  
Butyronitrile 110-59-8, Valeronitrile 140-75-0, 4-Fluorobenzylamine  
499-06-9, 3,5-Dimethylbenzoic acid 589-08-2, N-Methyl-2-phenylethylamine  
598-52-7, N-Methylthiourea 631-58-3, Thiopropionamide 645-45-4,  
3-Phenylpropionyl chloride 772-70-3, 3-(4-Fluorophenyl)propionyl  
chloride 873-32-5, 2-Chlorobenzonitrile 1194-02-1,  
4-Fluorobenzonitrile 1711-05-3, 3-Methoxybenzoyl chloride 1711-06-4,  
3-Methylbenzoyl chloride 2243-83-6, 2-Naphthoyl chloride 2393-23-9,  
4-Methoxybenzylamine 2627-86-3, (S)-1-Phenylethylamine 3886-69-9,  
(R)-1-Phenylethylamine 4152-90-3, 3-Chlorobenzylamine 4926-28-7,

2-Bromo-4-methylpyridine 5071-96-5, 3-Methoxybenzylamine 5271-67-0,  
2-Thiophenecarbonyl chloride 6850-57-3, 2-Methoxybenzylamine  
15893-42-2, 3-(4-Methoxyphenyl)propionyl chloride 18496-54-3,  
4-Phenylbutyryl chloride 20260-53-1, Nicotinoyl chloride hydrochloride  
20371-41-9, 5-Phenylvaleryl chloride 21382-98-9, 4-  
Methylthiobenzonitrile 27757-85-3, 2-Thienylmethylamine 90101-20-5,  
2-(tert-Butoxycarbonylamino)-4-methylpyridine

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor  
and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 461-87-0P, 2-Fluoro-4-methylpyridine 6613-44-1P, 3,5-Dimethylbenzoyl  
chloride 15717-17-6P, 2-Chlorothiobenzamide 16536-93-9P,  
Thiobutyramide 16536-94-0P, Thiovaleramide 21384-43-0P 22179-72-2P,  
4-Fluorothiobenzamide 53550-91-7P, 4-(Methylthio)thiobenzamide  
102336-06-1P 224040-60-2P 224040-71-5P 303162-27-8P 303162-28-9P  
303162-29-0P 303162-30-3P 303162-31-4P 303162-32-5P 303162-33-6P  
303162-34-7P 303162-35-8P 303162-36-9P 303162-37-0P 303162-38-1P  
303162-39-2P 303162-40-5P 303162-41-6P 303162-42-7P 303162-43-8P  
303162-44-9P 303162-45-0P 303162-46-1P 303162-47-2P 303162-48-3P  
303162-49-4P 303162-50-7P 303162-52-9P 303162-54-1P 303162-55-2P  
303162-56-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor  
and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

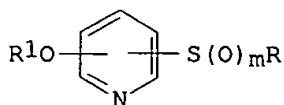
- (1) Merck & Co Inc; JP 11514353 A
- (2) Merck & Co Inc; CN 1203590 A CAPLUS
- (3) Merck & Co Inc; NZ 321738 A
- (4) Merck & Co Inc; US 5717100 A CAPLUS
- (5) Merck & Co Inc; EP 854870 A1 CAPLUS
- (6) Merck & Co Inc; AU 9675143 A CAPLUS
- (7) Merck & Co Inc; SK 9800435 A
- (8) Merck & Co Inc; CZ 9801043 A
- (9) Merck & Co Inc; NO 9801528 A CAPLUS
- (10) Merck & Co Inc; HU 9902294 A
- (11) Merck & Co Inc; WO 9712876 A1 1997 CAPLUS
- (12) Otsuka Pharmaceutical Co Ltd; JP 10152437 A CAPLUS
- (13) Otsuka Pharmaceutical Co Ltd; CN 1232396 A CAPLUS
- (14) Otsuka Pharmaceutical Co Ltd; EP 957915 A1 CAPLUS
- (15) Otsuka Pharmaceutical Co Ltd; BR 9712140 A CAPLUS
- (16) Otsuka Pharmaceutical Co Ltd; AU 9743221 A CAPLUS
- (17) Otsuka Pharmaceutical Co Ltd; WO 9814191 A1 1998 CAPLUS
- (18) Takeda Chemical Industries Ltd; JP 11193281 A CAPLUS
- (19) Takeda Chemical Industries Ltd; AU 9896480 A CAPLUS
- (20) Takeda Chemical Industries Ltd; WO 9921555 A2 1999 CAPLUS

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AN 1983:155211 CAPLUS  
 DN 98:155211  
 ED Entered STN: 12 May 1984  
 TI Sulfur-substituted phenoxypyridines having **antiviral** activity  
 IN Markley, Lowell D.; Tong, Yulan C.; Wood, Steven G.  
 PA Dow Chemical Co., USA  
 SO U.S., 22 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC A61K031-44; C07D021-263  
 NCL 424263000  
 CC 1-5 (Pharmacology)  
 Section cross-reference(s): 27  
 FAN.CNT 1

OK

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4371537	A	19830201	US 1981-292467	19810813
	ZA 8205762	A	19830629	ZA 1982-5762	19820809
	IL 66496	A1	19851129	IL 1982-66496	19820809
	CA 1180017	A1	19841225	CA 1982-409151	19820810
	EP 72529	A1	19830223	EP 1982-107263	19820811
	EP 72529	B1	19860129		
	R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
	GB 2103619	A1	19830223	GB 1982-23098	19820811
	GB 2103619	B2	19850227		
	AU 8287078	A1	19830512	AU 1982-87078	19820811
	AU 551683	B2	19860508		
	AT 17719	E	19860215	AT 1982-107263	19820811
	NO 8202751	A	19830214	NO 1982-2751	19820812
	NO 159851	B	19881107		
	NO 159851	C	19890215		
	DK 8203628	A	19830214	DK 1982-3628	19820812
	DK 157297	B	19891204		
	DK 157297	C	19900507		
	JP 58041868	A2	19830311	JP 1982-139277	19820812
	JP 04014107	B4	19920311		
	ES 514940	A1	19831016	ES 1982-514940	19820812
	ES 523661	A1	19850316	ES 1983-523661	19830628
	ES 523660	A1	19850401	ES 1983-523660	19830628
PRAI	US 1981-292467		19810813		
	EP 1982-107263		19820811		
OS	CASREACT 98:155211				
GI					



AB The title compds. I [R = C1-7 alkyl, C5 or C6 cycloalkyl, Ar(CH<sub>2</sub>)<sub>q</sub> (Ar = C6-10 aryl, q = 0-3), R1 = Ph or substituted Ph; m = 0, 1, or 2] preferably administered as pharmaceutical compns. (no data given) were prepd. by several methods and evaluated as **antiviral** agents. Thus, 2-(3,4-dichlorophenoxy)-5-(methylsulfonyl)pyridine [85331-30-2] prepd. by the reaction of 3,4-dichlorophenol [95-77-2] in DMSO in presence of Na tert-butoxide with 2,5-bis(methylsulfonyl)pyridine showed a



broad spectrum **antiviral** activity at low conc. (25 .mu.g/mL).

ST phenoxythiopyridine prepn **antiviral**; virucide  
 phenoxythiopyridine; pyridine phenoxythio prepn **antiviral**

IT Virucides and Virustats  
 (phenoxythiopyridines)

IT 85330-61-6P 85330-67-2P 85330-70-7P 85330-73-0P **85330-76-3P**  
 85331-31-3P 85331-32-4P 85331-38-0P 85331-39-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and decarboxylation of)

IT 85331-36-8P 85331-37-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and hydrolysis of)

IT 58819-71-9P 71506-85-9P 85330-62-7P 85330-65-0P 85330-68-3P  
 85330-69-4P 85330-71-8P 85330-74-1P **85330-77-4P**  
 85330-81-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and oxidn. of)

IT 85331-34-6P 85331-35-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with dichlorophenol)

IT 85330-72-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with hydroxyacetophenone)

IT **85330-78-5P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with hydroxybenzophenone)

IT 25935-30-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with sodium methanethiolate)

IT 85330-63-8P 85330-64-9P 85330-66-1P 85330-75-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with substituted phenols)

IT 25935-29-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and redn. of)

IT 85330-84-3P 85330-85-4P 85330-86-5P 85330-87-6P 85330-88-7P  
 85330-89-8P 85330-90-1P 85330-91-2P 85330-92-3P 85330-93-4P  
 85330-94-5P 85330-95-6P 85330-96-7P 85330-97-8P 85330-98-9P  
 85330-99-0P 85331-00-6P 85331-01-7P 85331-02-8P 85331-03-9P  
 85331-04-0P 85331-05-1P 85331-06-2P 85331-07-3P 85331-08-4P  
 85331-09-5P 85331-10-8P 85331-11-9P 85331-12-0P 85331-13-1P  
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 85331-24-4P 85331-25-5P 85331-26-6P 85331-27-7P 85331-28-8P  
 85331-29-9P 85331-30-2P 85345-64-8P 85368-98-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and virucidal activity)

IT 62916-42-1P 85330-79-6P 85330-80-9P 85330-82-1P 85330-83-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

IT 75-33-2  
 RL: BIOL (Biological study)  
 (reaction of with Me dichloropyridinecarboxylate)

IT 100-53-8 108-98-5, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with Me dichloropyridinecarboxylate)

IT 95-95-4 533-31-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with bis(ethylsulfonyl)pyridine)

IT 98-54-4 99-93-4 101-53-1 106-41-2 106-48-9 461-84-7 591-20-8  
 767-00-0 831-82-3 873-62-1 1073-72-9 1137-42-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with bis(methylsulfonyl)pyridine)

IT 95-77-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with chloronitropyridine)

IT 140-89-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with diazotized pyridine derivs.)

IT 4548-45-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with dichlorophenol)

IT 1569-69-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with dichloropyridinecarboxylic acid)

IT 75-08-1 111-31-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with dichloropyridinecarboxylic acid)

IT 1532-24-7 1702-17-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with mercaptans)

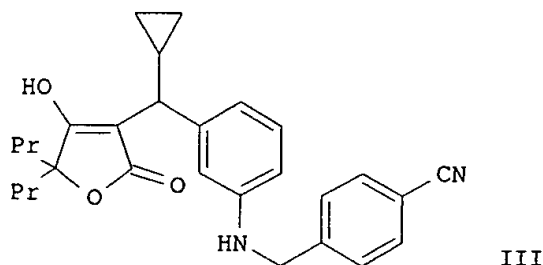
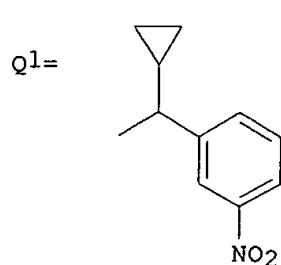
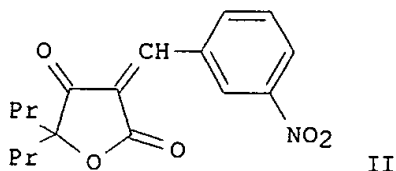
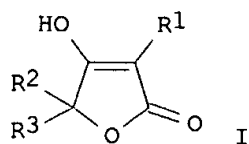
IT 26452-80-2 85331-33-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with methanethiol)

IT 74-93-1, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with pyridinecarboxylates)

=>

AN 1999:705001 CAPLUS  
 DN 131:322530  
 ED Entered STN: 04 Nov 1999  
 TI Substituted tetronic acids useful for treating HIV and other retroviruses  
 IN Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin, James M.; Smith, Clark W.; Tommasi, Ruben A.; Aristoff, Paul A.; Skulnick, Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.  
 PA USA  
 SO U.S., 116 pp., Cont.-in-part of U.S. Ser. No. 238,820, abandoned.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A61K031-34  
 ICS A61K031-335; A61K031-415; A61K031-505  
 NCL 514473000  
 CC 27-6 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 1  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5977169	A	19991102	US 1997-604937	19970728
	ZA 9406099	A	19960212	ZA 1994-6099	19940812
	WO 9507901	A1	19950323	WO 1994-US9533	19940907
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
	RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
PRAI	US 1993-123029		19930917		
	US 1994-238820		19940506		
	WO 1994-US9533		19940907		
OS	MARPAT 131:322530				
GI					



AB The invention comprises novel substituted tetronic acid derivs. (I) and tautomers [wherein R1-R3 = wide variety of specified C-contg. substituents] that are inhibitors of HIV protease. I retard replication of any retrovirus contg. aspartyl protease and are

useful for treatment of AIDS or AIDS-related diseases. Approx. 250 compds. are claimed, and phys. and biol. data for approx. 120 compds. are provided. For example, condensation of I [R1 = H, R2 = R3 = Pr] with 3-nitrobenzaldehyde gave >100% crude nitrobenzylidene deriv. II, which reacted with cyclopropylmagnesium bromide and CuBr.SMe2 in THF to give 62% I [R1 = Q1, R2 = R3 = Pr]. Hydrogenation of the nitro group (97%) and sulfonamidation of the resultant amino group with 4-cyanobenzenesulfonyl chloride (53%) gave title furandione III, a preferred compd. Several compds. including III are said to have inhibited replication of HIV-1IIIB in human cell lines. HIV-1 protease inhibitory data are provided, and over 100% inhibition was reported for many test compds. at doses as low as 3.3 .mu.M.

ST tetronic acid prepn antiviral **retrovirus** replication inhibitor;  
furandione prepn antiviral **retrovirus** replication inhibitor;  
HIV protease inhibitor AIDS treatment tetronic acid prepn

IT Human immunodeficiency virus  
Human immunodeficiency virus 1  
(inhibition; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT Anti-AIDS agents  
Antiviral agents  
(prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT AIDS (disease)  
(treatment; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 144114-21-6, Retropepsin  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(inhibitors; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 1138-44-9P 10424-93-8P 72036-34-1P 85520-35-0P 161720-04-3P  
164346-90-1P 164346-91-2P 164346-92-3P 164346-93-4P 164346-94-5P  
164346-95-6P 164346-96-7P 164346-98-9P 164346-99-0P 164347-01-7P  
164347-02-8P 164347-03-9P 164347-07-3P 164347-10-8P 248608-58-4P  
248608-59-5P 248608-60-8P 248608-61-9P 248608-62-0P 248608-63-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 99-61-6, 3-Nitrobenzaldehyde 100-39-0, Benzyl bromide 103-63-9, (2-Bromoethyl)benzene 104-53-0, Hydrocinnamaldehyde 106-94-5  
108-94-1, Cyclohexanone, reactions 109-72-8, n-Butyl lithium, reactions 120-92-3, Cyclopentanone 502-49-8, Cyclooctanone 623-47-2, Ethyl propiolate 637-59-2, 1-Bromo-3-phenylpropane 946-33-8, 2-Benzylcyclohexanone 1007-03-0, .alpha.-Cyclopropylbenzyl alcohol 1067-74-9, Methyl diethylphosphonoacetate 2550-26-7, Benzyl acetone 2637-37-8, 2-Quinolinethiol 4423-94-3, 2-Ethylcyclohexanone 4971-56-6, Tetronic acid 14371-10-9 23719-80-4, Cyclopropylmagnesium bromide 29976-53-2, 1-Carbethoxy-4-piperidone 49584-26-1, 4-Cyanobenzenesulfonyl chloride 118753-70-1 135005-10-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 164344-46-1P 164344-47-2P 164344-48-3P 164344-49-4P 164344-50-7P  
164344-51-8P 164344-52-9P 164344-53-0P 164344-54-1P 164344-55-2P  
164344-56-3P 164344-57-4P 164344-58-5P 164344-59-6P 164344-60-9P  
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164344-71-2P 164344-72-3P 164344-73-4P 164344-74-5P 164344-75-6P  
164344-76-7P 164344-77-8P 164344-79-0P 164344-80-3P 164344-81-4P  
164344-82-5P 164344-83-6P 164344-84-7P 164344-85-8P 164344-86-9P  
164344-87-0P 164344-88-1P 164344-89-2P 164344-90-5P 164344-91-6P

164344-92-7P	164344-93-8P	164344-94-9P	164344-96-1P	164344-97-2P
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248608-40-4P	248608-41-5P	248608-42-6P	248608-43-7P	248608-44-8P
248608-45-9P				

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(target compd.; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 248608-46-0P 248608-48-2P 248608-49-3P 248608-50-6P 248608-51-7P  
248608-52-8P 248608-53-9P 248608-54-0P 248608-56-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(target compd.; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

- (1) Anderson, J; JCS Perkin 1 1982, V1, P215
- (2) Anon
- (3) Anon; 1963
- (4) Anon; 1965
- (5) Anon; 1977 CAPLUS
- (6) Anon; 1979 CAPLUS
- (7) Anon; 1979 CAPLUS

- (8) Anon; 1979 CAPLUS  
(9) Anon; 1982 CAPLUS  
(10) Anon; 1983 CAPLUS  
(11) Anon; EP 0202589 A2 1986 CAPLUS  
(12) Anon; EP 0259707 1988 CAPLUS  
(13) Anon; EP 0365329 1990 CAPLUS  
(14) Anon; JP 04-211676 1992 CAPLUS  
(15) Anon; EP 0480624 A1 1992 CAPLUS  
(16) Anon; 1993 CAPLUS  
(17) Anon; JP 05-043568 1993 CAPLUS  
(18) Anon; EP 0534907 1993 CAPLUS  
(19) Anon; WO 9304055 1993 CAPLUS  
(20) Anon; WO 9411361 1994 CAPLUS  
(21) Anon; J Synthetic Org Chem 1986, V44(2), P127  
(22) Arai, K; Chem Pharm Bull 1989, V37(12), P3229 CAPLUS  
(23) Buck, J; J Chem Soc Perkin Trans 1985, V1, P2399  
(24) Damon, R; Tetrahedron Letters 1976, 32, P2749 CAPLUS  
(25) Fell, S; JCS Chem Comm 1979, P81 CAPLUS  
(26) Gudgeon, J; Bioorganic Chemistry 1979, V8, P311 CAPLUS  
(27) Gudgeon, J; JCS Chem Commun 1974, P636 CAPLUS  
(28) Lang, M; Arch Pharm 1993, V326, P921 CAPLUS  
(29) Rehse, K; Arch Pharm 1978, V311, P986 CAPLUS  
(30) Rehse, K; Arch Pharm 1979, V312, P164 CAPLUS  
(31) Rehse, K; Arch Pharm 1982, V315, P052 CAPLUS  
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(35) Sudo, R; J Org Chem V32(6), P1844 CAPLUS  
(36) Vekemans, J; Tetrahedron Letters 1987, V28(20), P2299 CAPLUS  
(37) Wakabayashi, H; Chemistry Letters 1987, P875  
(38) Wanwagenen, B; Tetrahedron 1986, V42(4), P1117

=>

AN 1997:165733 CAPLUS  
DN 126:258470  
ED Entered STN: 12 Mar 1997  
TI Synthesis and pharmacological evaluation of sulfone substituted  
HIV protease inhibitors  
AU Schwartz, Theresa M.; Bundy, Gordon L.; Strohbach, Joseph W.;  
Thairrivongs, Suvit; Johnson, Paul D.; Skulnick, Harvey I.; Tomich, Paul  
K.; Lynn, Janet C.; Chong, Kong Teck; Hinshaw, Roger R.; Raub, Thomas J.;  
Padbury, Guy E.; Loth, Lisa N.  
CS Res. Labs., Pharmacia Upjohn, Inc., Kalamazoo, MI, 49001-0199, USA  
SO Bioorganic & Medicinal Chemistry Letters (1997), 7(4), 399-402  
CODEN: BMCLE8; ISSN: 0960-894X  
PB Elsevier  
DT Journal  
LA English  
CC 1-3 (Pharmacology)  
AB The sulfonamide substituted pyranones (1) have recently been shown to be  
potent HIV protease inhibitors. We prepared a series of sulfone  
substituted analogs and compared and their biol. activities to those of  
the corresponding sulfonamide analogs. It was detd. that although these  
compds. maintained activity as enzyme inhibitors, they showed somewhat  
diminished antiviral activity event though they may possess increased  
membrane permeability.  
ST sulfonamide pyranone prepn HIV protease inhibitor  
IT Structure-activity relationship  
(antiviral; sulfonamide substituted pyranones as HIV protease  
inhibitors)  
IT Structure-activity relationship  
(aspartic proteinase-inhibiting; sulfonamide substituted pyranones as  
HIV protease inhibitors)  
IT Anti-AIDS agents  
Antiviral agents  
Human immunodeficiency virus 1  
(sulfonamide substituted pyranones as HIV protease  
inhibitors)  
IT 174483-90-0  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); BIOL (Biological study)  
(antiviral and HIV-1 protease inhibiting activity of)  
IT 166335-18-8P 166335-24-6P 166335-32-6P 166335-74-6P 166335-80-4P  
174483-25-1P 174483-26-2P 174483-27-3P 174483-28-4P 174483-29-5P  
174483-30-8P 174483-56-8P 174483-62-6P 174483-63-7P 174483-94-4P  
**188839-13-6P** 188839-14-7P 188839-15-8P **188839-16-9P**  
188839-17-0P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); BIOL (Biological  
study); PREP (Preparation)  
(prepn. and antiviral and HIV-1 protease inhibiting activity  
of)  
IT 162174-73-4P 174484-94-7P 188839-19-2P 188839-20-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reaction of)  
IT 675-10-5 7051-34-5, Bromomethyl cyclopropane 100058-82-0 174484-93-6  
188839-18-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of)  
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE  
(1) Chong, K; Antimicrob Agents Chemother 1994, V38, P288 CAPLUS  
(2) Conradi, R; Pharm Res 1991, V8, P1453 CAPLUS  
(3) Nogami, H; Chem Pharm Bull 1968, V16, P580 CAPLUS

- (4) Raub, T; Unpublished result
- (5) Romines, K; Curr Med Chem 1995, V2, P825 CAPLUS
- (6) Romines, K; J Med Chem 1995, V38, P4463 CAPLUS
- (7) Sawada, G; Pharm Res 1994, V11, P665 CAPLUS
- (8) Skulnick, H; J Med Chem 1995, V38, P4968 CAPLUS
- (9) Skulnick, H; J Med Chem, in press
- (10) Thaisrivongs, S; J Med Chem 1994, V37, P3200 CAPLUS
- (11) Thaisrivongs, S; J Med Chem 1996, V39, P2400 CAPLUS



O=C1C(=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3)C(=O)OC1C(C2)C(C2)C3

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

NOTICE SET TO OFF FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

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AN 2002:974259 CAPLUS  
 DN 138:33310  
 ED Entered STN: 26 Dec 2002  
 TI Antiretroviral compounds and compositions  
 IN Brewer, Arthur D.; Cantor, Stephen E.; Dekeyser, Mark A.; Doweiko, Arthur  
 M. P.; Harris, John W.; Lacadie, John A.; Pierce, James B.; Mary, Louise  
 Jones Howard L.; Harrison, William A.  
 PA Uniroyal Chemical Company, Inc., USA  
 SO U.S., 19 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A61K031-47  
 ICS C07D215-16; C07D211-72; C07D211-84  
 NCL 546157000; 546290000; 546294000; 514312000; 514345000; 514347000  
 CC 1-5 (Pharmacology)  
 Section cross-reference(s): 27

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6498254	B1	20021224	US 2001-21202	20011029
	WO 2003037866	A1	20030508	WO 2002-US29573	20020917
	W: AU, BR, CA, CN, JP, MX				
PRAI	US 2001-21202	A	20011029		
AB	Certain pyridine and quinoline derivs. which inhibit replication of the retroviruses HIV-1, HIV-2 and human cytomegalovirus (HCMV) are provided. Pharmaceutical compns. useful in methods of treating or inhibiting certain retrovirus infections are described.				
ST	antiretroviral compd pyridine quinoline deriv				
IT	Anti-AIDS agents				
	Antiviral agents				
	Human				
	Human herpesvirus 5				
	Human immunodeficiency virus 1				
	Human immunodeficiency virus 2				
	(antiretroviral compds. and compns. using pyridine and quinoline derivs.)				
IT	Drug delivery systems				
	(carriers; antiretroviral compds. and compns. using pyridine and quinoline derivs.)				
IT	478620-19-8P	478620-24-5P	478620-25-6P	478620-28-9P	
	RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)				
	(antiretroviral compds. and compns. using pyridine and quinoline derivs.)				
IT	69212-31-3P, 2-Benzylthio-3-nitropyridine	478619-45-3P	478619-49-7P		
	478619-53-3P	478619-57-7P	478619-61-3P	478619-65-7P	478619-68-0P
	478619-72-6P	478619-78-2P	478619-82-8P	478619-86-2P	478619-90-8P
	478619-94-2P	478619-98-6P	478620-02-9P	478620-06-3P	478620-08-5P
	478620-11-0P	478620-12-1P	478620-14-3P	478620-16-5P	478620-18-7P
	478620-20-1P	478620-21-2P	478620-23-4P	478620-26-7P	478620-27-8P
	478620-29-0P	478620-30-3P	478620-31-4P	478620-32-5P	478620-33-6P
	478620-34-7P	478620-35-8P	478620-36-9P	478620-37-0P	478620-38-1P
	478620-39-2P				
	RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)				
	(antiretroviral compds. and compns. using pyridine and quinoline derivs.)				
IT	51-79-6, Urethane	86-81-7, 3,4,5-Trimethoxybenzaldehyde	100-44-7,		
	Benzyl chloride, reactions	100-52-7, Benzaldehyde, reactions	100-53-8,		

Benzylmercaptan 123-11-5, 4-Methoxybenzaldehyde, reactions 607-66-9,  
 2-Hydroxy-4-methylquinoline 824-45-3, 2,5-Dimethylbenzyl chloride  
 2014-83-7, 2,6-Dichlorobenzyl chloride 2044-27-1, 1-Methyl-2(1H)-  
 pyridinethione 2587-00-0, 2,6-Dichloropyridine-N-oxide 2637-34-5,  
 2-Mercaptopyridine 3811-73-2 5470-18-8, 2-Chloro-3-nitropyridine  
 6258-60-2, 4-Methoxybenzylmercaptan 20871-93-6 22182-98-5  
 52694-50-5, 3-Chloromethyl-1-methylpiperidine 53976-62-8 53976-65-1  
 60263-88-9 82959-54-4 84504-48-3 91668-83-6, 2-Chloro-3-  
 methylpyridine-N-oxide 338778-95-3 478619-47-5 478619-51-1  
 478619-55-5 478619-59-9 478619-63-5 478619-70-4  
 478619-76-0 478619-80-6 478619-84-0 478619-88-4 478619-92-0  
 478619-96-4 478620-00-7 478620-05-2 478620-07-4 478620-09-6  
 478620-10-9 478620-13-2 478620-15-4 478620-17-6 478620-22-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(antiretroviral compds. and compns. using pyridine and quinoline  
 derivs.)

IT 4437-65-4P 81167-65-9P 81167-66-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(antiretroviral compds. and compns. using pyridine and quinoline  
 derivs.)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE

- (1) Brouwer; US 5696151 A 1997 CAPLUS
- (2) Harrison; US 5268389 A 1993 CAPLUS
- (3) Moormann; US 5945425 A 1999 CAPLUS

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present  
NEWS 4 DEC 08 INPADOC: Legal Status data reloaded  
NEWS 5 SEP 29 DISSABS now available on STN  
NEWS 6 OCT 10 PCTFULL: Two new display fields added  
NEWS 7 OCT 21 BIOSIS file reloaded and enhanced  
NEWS 8 OCT 28 BIOSIS file segment of TOXCENTER reloaded and enhanced  
NEWS 9 NOV 24 MSDS-CCOHS file reloaded  
NEWS 10 DEC 08 CABA reloaded with left truncation  
NEWS 11 DEC 08 IMS file names changed  
NEWS 12 DEC 09 Experimental property data collected by CAS now available  
in REGISTRY  
NEWS 13 DEC 09 STN Entry Date available for display in REGISTRY and CA/CAPLUS  
NEWS 14 DEC 17 DGENE: Two new display fields added  
NEWS 15 DEC 18 BIOTECHNO no longer updated  
NEWS 16 DEC 19 CROPU no longer updated; subscriber discount no longer  
available  
NEWS 17 DEC 22 Additional INPI reactions and pre-1907 documents added to CAS  
databases  
NEWS 18 DEC 22 IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields  
NEWS 19 DEC 22 ABI-INFORM now available on STN  
  
NEWS EXPRESS DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT  
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003  
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=> file reg

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SINCE FILE

TOTAL

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ENTRY

SESSION

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DICTIONARY FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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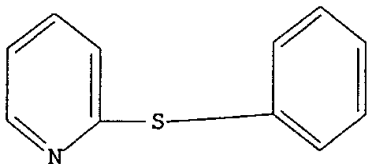
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L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 exa sam

SAMPLE SEARCH INITIATED 09:20:47 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 25 TO ITERATE

100.0% PROCESSED 25 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 200 TO 800

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA EXA SAM L1

=> s l1 fam sam

SAMPLE SEARCH INITIATED 09:21:01 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 56 TO ITERATE

100.0% PROCESSED 56 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 672 TO 1568  
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA FAM SAM L1

=> s l1 sss sam

SAMPLE SEARCH INITIATED 09:21:16 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 552 TO ITERATE

100.0% PROCESSED 552 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

50 ANSWERS

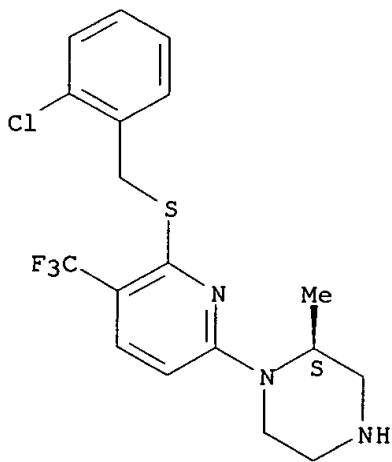
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 9631 TO 12449  
PROJECTED ANSWERS: 3098 TO 4782

L4 50 SEA SSS SAM L1

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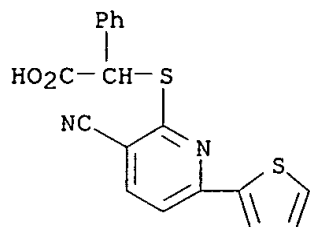
L4 ANSWER 1 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 625844-46-4 REGISTRY  
CN Piperazine, 1-[6-[[[2-chlorophenyl)methyl]thio]-5-(trifluoromethyl)-2-  
pyridinyl]-2-methyl-, (2S)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C18 H19 Cl F3 N3 S  
CI COM  
SR CA

Absolute stereochemistry.



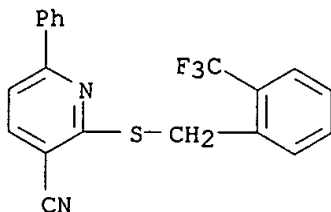
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 2 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 625375-04-4 REGISTRY  
 CN Benzeneacetic acid, .alpha.-[[3-cyano-6-(2-thienyl)-2-pyridinyl]thio]-  
 (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C18 H12 N2 O2 S2  
 SR Chemical Library  
 LC STN Files: CHEMCATS



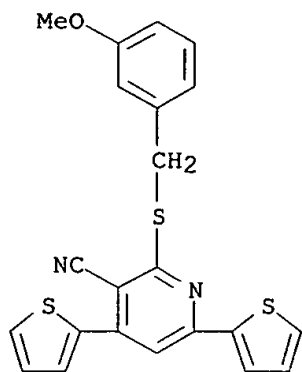
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L4 ANSWER 3 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 625371-98-4 REGISTRY  
 CN 3-Pyridinecarbonitrile, 6-phenyl-2-[[[2-(trifluoromethyl)phenyl]methyl]thio]-  
 (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C20 H13 F3 N2 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



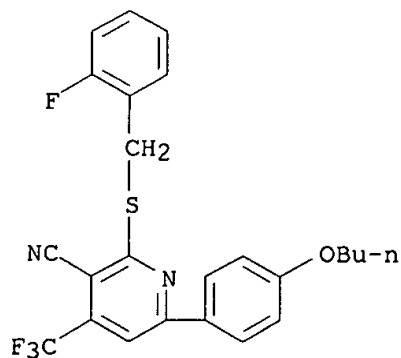
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L4 ANSWER 4 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 625371-35-9 REGISTRY  
 CN 3-Pyridinecarbonitrile, 2-[[[3-methoxyphenyl]methyl]thio]-4,6-di-2-thienyl-  
 (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C22 H16 N2 O S3  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

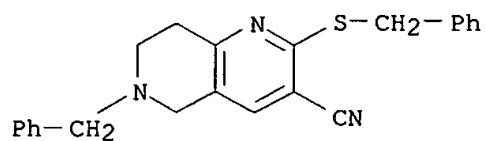
L4 ANSWER 5 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 608494-96-8 REGISTRY  
 CN 3-Pyridinecarbonitrile, 6-(4-butoxyphenyl)-2-[[2-fluorophenyl)methyl]thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)  
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 MF C24 H20 F4 N2 O S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



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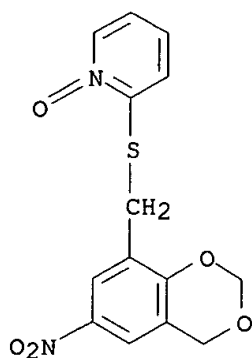
L4 ANSWER 6 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 607698-12-4 REGISTRY  
 CN 1,6-Naphthyridine-3-carbonitrile, 5,6,7,8-tetrahydro-6-(phenylmethyl)-2-[[2-(phenylmethyl)thio]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C23 H21 N3 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS





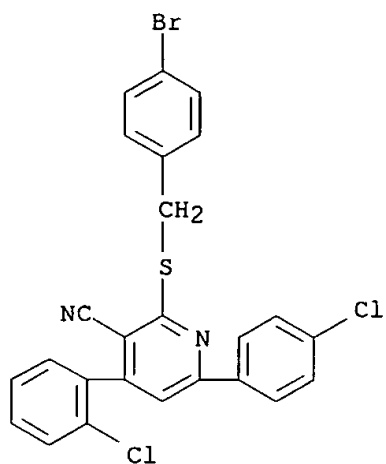
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L4 ANSWER 7 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 556022-40-3 REGISTRY  
 CN Pyridine, 2-[[6-nitro-4H-1,3-benzodioxin-8-yl)methyl]thio]-, 1-oxide  
 (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C14 H12 N2 O5 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



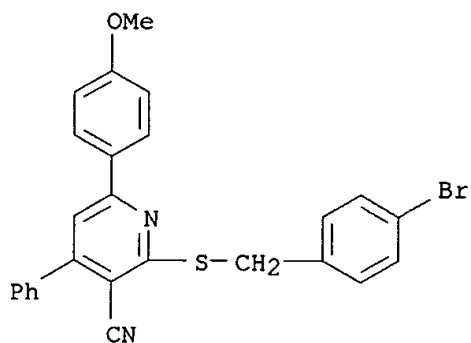
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L4 ANSWER 8 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 553658-94-9 REGISTRY  
 CN 3-Pyridinecarbonitrile, 2-[[4-bromophenyl)methyl]thio]-4-(2-chlorophenyl)-  
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 FS 3D CONCORD  
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 SR Chemical Library  
 LC STN Files: CHEMCATS



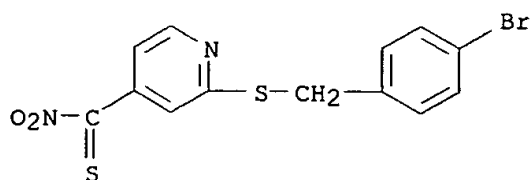
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L4 ANSWER 9 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
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 SR Chemical Library  
 LC STN Files: CHEMCATS



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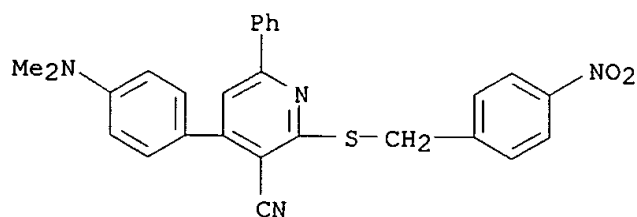
L4 ANSWER 10 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 537656-95-4 REGISTRY  
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 SR CA  
 LC STN Files: CA, CAPLUS



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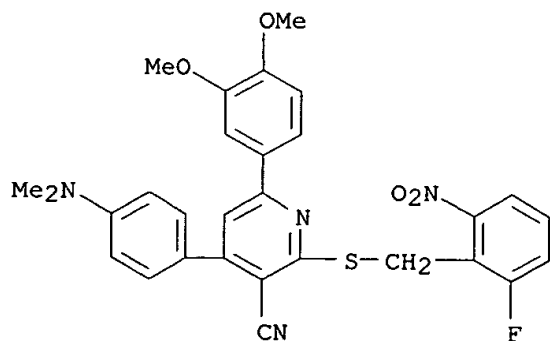
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 11 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 514853-30-6 REGISTRY  
CN 3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-2-[[4-nitrophenyl)methyl]thio]-6-phenyl- (9CI) (CA INDEX NAME)  
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MF C27 H22 N4 O2 S  
SR Chemical Library  
LC STN Files: CHEMCATS



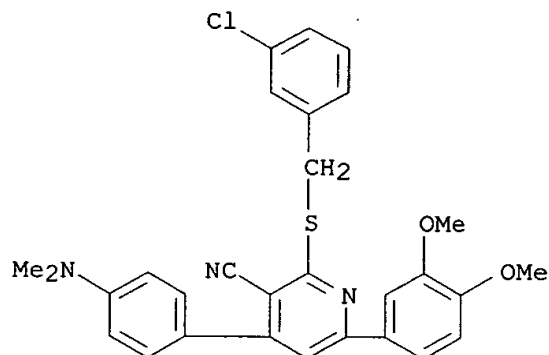
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 12 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 514852-33-6 REGISTRY  
CN 3-Pyridinecarbonitrile, 6-(3,4-dimethoxyphenyl)-4-[4-(dimethylamino)phenyl]-2-[[2-fluoro-6-nitrophenyl)methyl]thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C29 H25 F N4 O4 S  
SR Chemical Library  
LC STN Files: CHEMCATS



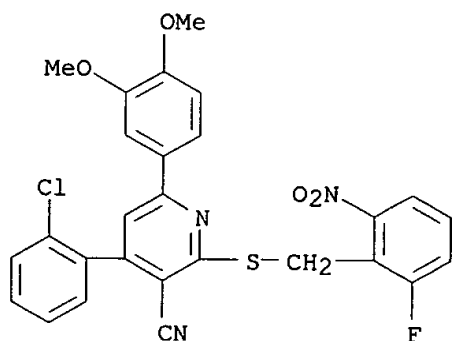
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 13 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 514851-98-0 REGISTRY  
CN 3-Pyridinecarbonitrile, 2-[[ (3-chlorophenyl)methyl]thio]-6-(3,4-dimethoxyphenyl)-4-[4-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C29 H26 Cl N3 O2 S  
SR Chemical Library  
LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

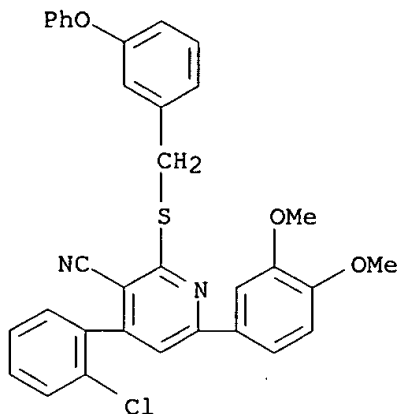
L4 ANSWER 14 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 514851-49-1 REGISTRY  
CN 3-Pyridinecarbonitrile, 4-(2-chlorophenyl)-6-(3,4-dimethoxyphenyl)-2-[[ (2-fluoro-6-nitrophenyl)methyl]thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C27 H19 Cl F N3 O4 S  
SR Chemical Library  
LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

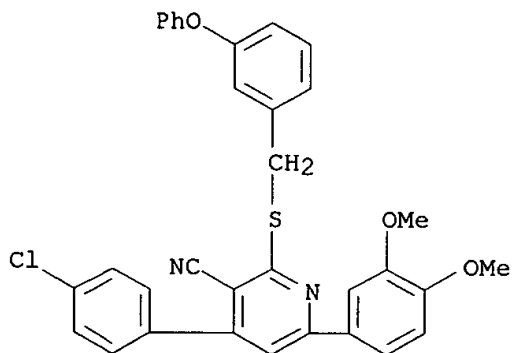
L4 ANSWER 15 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 514851-39-9 REGISTRY

CN 3-Pyridinecarbonitrile, 4-(2-chlorophenyl)-6-(3,4-dimethoxyphenyl)-2-[[ (3-phenoxyphenyl)methyl]thio]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C33 H25 Cl N2 O3 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

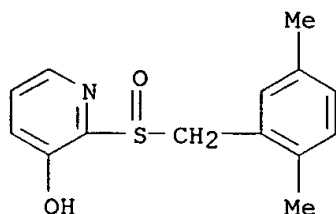
L4 ANSWER 16 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 514850-93-2 REGISTRY  
 CN 3-Pyridinecarbonitrile, 4-(4-chlorophenyl)-6-(3,4-dimethoxyphenyl)-2-[[ (3-phenoxyphenyl)methyl]thio]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C33 H25 Cl N2 O3 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 17 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 500163-27-9 REGISTRY  
 CN 3-Pyridinol, 2-[[ (2,5-dimethylphenyl)methyl]sulfinyl]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C14 H15 N O2 S

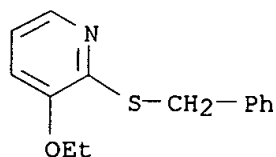
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

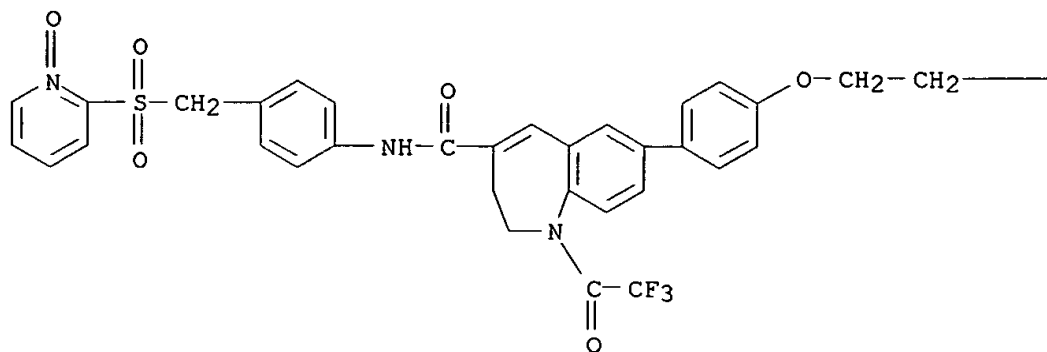
L4 ANSWER 18 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 500163-13-3 REGISTRY  
CN Pyridine, 3-ethoxy-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C14 H15 N O S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 19 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 497851-00-0 REGISTRY  
CN 1H-1-Benzazepine-4-carboxamide, 7-[4-(2-butoxyethoxy)phenyl]-2,3-dihydro-N-[4-[[[(1-oxido-2-pyridinyl)sulfonyl]methyl]phenyl]-1-(trifluoroacetyl)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C37 H36 F3 N3 O7 S  
SR CA  
LC STN Files: CA, CAPLUS



— OBU-n

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 20 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN

RN 497246-37-4 REGISTRY

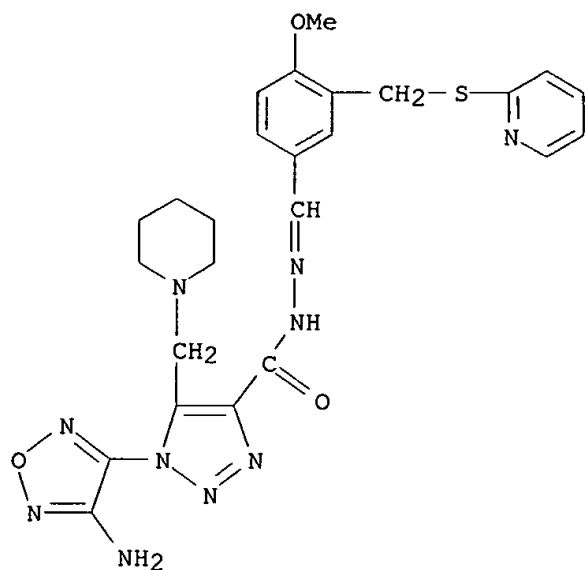
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(4-amino-1,2,5-oxadiazol-3-yl)-5-(1-piperidinylmethyl)-, [[4-methoxy-3-[(2-pyridinylthio)methyl]phenyl]methyle ne]hydrazide (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C25 H28 N10 O3 S

SR Chemical Library

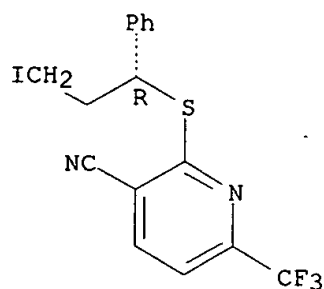
LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 21 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 496871-24-0 REGISTRY  
 CN 3-Pyridinecarbonitrile, 2-[[[(1R)-3-iodo-1-phenylpropyl]thio]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C16 H12 F3 I N2 S  
 SR CA  
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

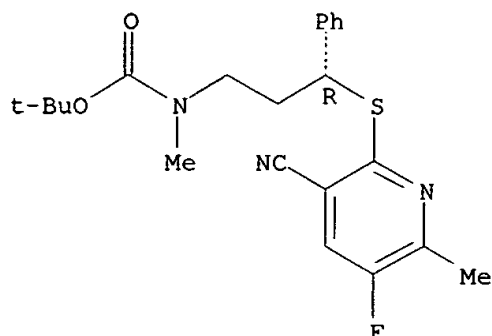
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 22 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 496871-22-8 REGISTRY  
 CN Carbamic acid, [(3R)-3-[(3-cyano-5-fluoro-6-methyl-2-pyridinyl)thio]-3-phenylpropyl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C22 H26 F N3 O2 S  
 SR CA



LC STN Files: CA, CAPLUS

Absolute stereochemistry.

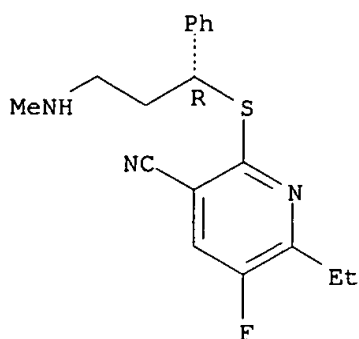


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 23 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 496870-29-2 REGISTRY  
CN 3-Pyridinecarbonitrile, 6-ethyl-5-fluoro-2-[(1R)-3-(methylamino)-1-phenylpropyl]thio]-, dihydrochloride (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C18 H20 F N3 S . 2 Cl H  
SR CA  
LC STN Files: CA, CAPLUS  
CRN (496870-54-3)

Absolute stereochemistry.

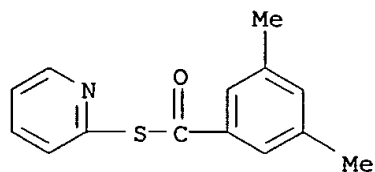


● 2 HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 24 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 496067-45-9 REGISTRY  
CN Benzenecarbothioic acid, 3,5-dimethyl-, S-2-pyridinyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD

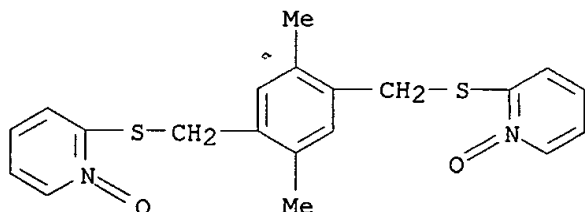
MF C14 H13 N O S  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

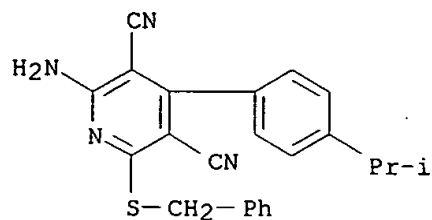
L4 ANSWER 25 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 478619-55-5 REGISTRY  
CN Pyridine, 2,2'-[(2,5-dimethyl-1,4-phenylene)bis(methylenethio)]bis-,  
1,1'-dioxide (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C20 H20 N2 O2 S2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

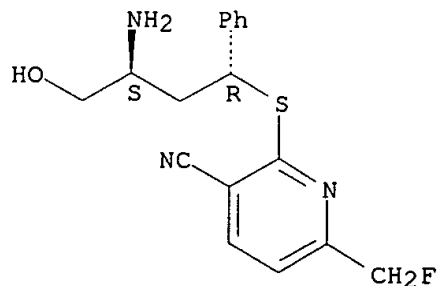
L4 ANSWER 26 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 476319-21-8 REGISTRY  
CN 3,5-Pyridinedicarbonitrile, 2-amino-4-[4-(1-methylethyl)phenyl]-6-  
[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H20 N4 S  
SR Chemical Library  
LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 27 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 474823-65-9 REGISTRY  
 CN 3-Pyridinecarbonitrile, 2-[[{(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-6-(fluoromethyl)- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN 2-[[{(1R,3S)-3-Amino-4-hydroxy-1-phenylbutyl]thio]-6-(fluoromethyl)-3-pyridinecarbonitrile  
 FS STEREOSEARCH  
 MF C17 H18 F N3 O S  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS

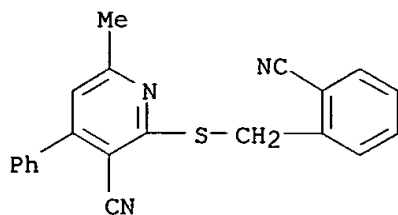
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

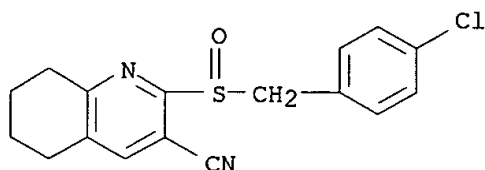
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 28 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 459182-40-2 REGISTRY  
 CN 3-Pyridinecarbonitrile, 2-[[{(2-cyanophenyl)methyl]thio]-6-methyl-4-phenyl- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C21 H15 N3 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



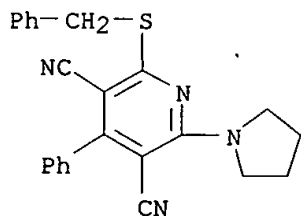
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 29 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 459154-94-0 REGISTRY  
 CN 3-Quinolinecarbonitrile, 2-[(4-chlorophenyl)methyl]sulfinyl]-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C17 H15 Cl N2 O S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

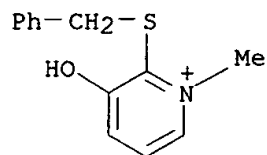
L4 ANSWER 30 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 455877-30-2 REGISTRY  
 CN 3,5-Pyridinedicarbonitrile, 4-phenyl-2-[(phenylmethyl)thio]-6-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C24 H20 N4 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

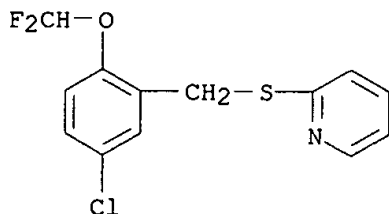
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 31 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 454421-81-9 REGISTRY  
 CN Pyridinium, 3-hydroxy-1-methyl-2-[(phenylmethyl)thio]-, bromide (9CI) (CA INDEX NAME)  
 MF C13 H14 N O S . Br  
 SR Chemical Library  
 LC STN Files: CHEMCATS



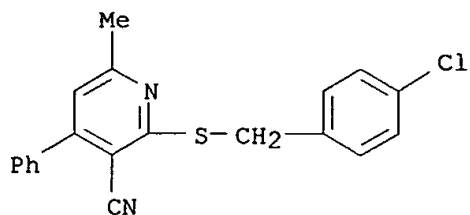
● Br<sup>-</sup>

L4 ANSWER 32 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 452299-62-6 REGISTRY  
 CN Pyridine, 2-[[[5-chloro-2-(difluoromethoxy)phenyl]methyl]thio]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C13 H10 Cl F2 N O S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



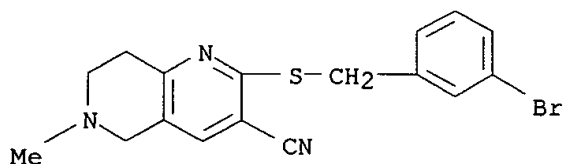
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 33 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 449748-57-6 REGISTRY  
 CN 3-Pyridinecarbonitrile, 2-[[[4-chlorophenyl]methyl]thio]-6-methyl-4-phenyl- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C20 H15 Cl N2 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



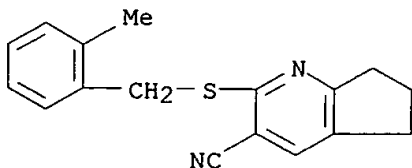
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 34 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 445383-68-6 REGISTRY  
 CN 1,6-Naphthyridine-3-carbonitrile, 2-[[3-(4-bromophenyl)methyl]thio]-5,6,7,8-tetrahydro-6-methyl- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C17 H16 Br N3 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

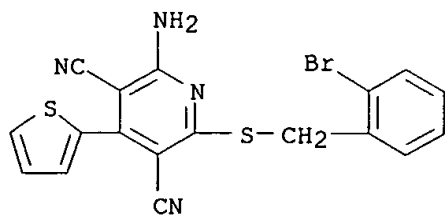
L4 ANSWER 35 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 445383-65-3 REGISTRY  
 CN 5H-Cyclopenta[b]pyridine-3-carbonitrile, 6,7-dihydro-2-[[2-(4-bromophenyl)methyl]thio]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C17 H16 N2 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

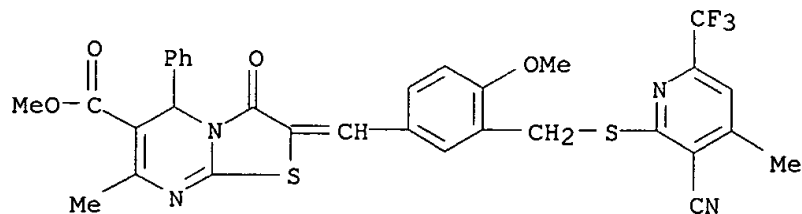
L4 ANSWER 36 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 445381-37-3 REGISTRY  
 CN 3,5-Pyridinedicarbonitrile, 2-amino-6-[[2-(4-bromophenyl)methyl]thio]-4-(2-thienyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD  
 MF C18 H11 Br N4 S2  
 SR Chemical Library  
 LC STN Files: CHEMCATS



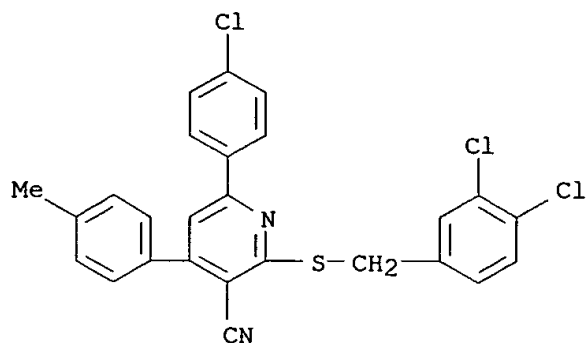
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 37 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 445244-89-3 REGISTRY  
 CN 5H-Thiazolo[3,2-a]pyrimidine-6-carboxylic acid, 2-[[[3-cyano-4-methyl-6-(trifluoromethyl)-2-pyridinyl]thio]methyl]-4-methoxyphenyl]methylene]-2,3-dihydro-7-methyl-3-oxo-5-phenyl-, methyl ester (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C32 H25 F3 N4 O4 S2  
 SR Chemical Library  
 LC STN Files: CHEMCATS



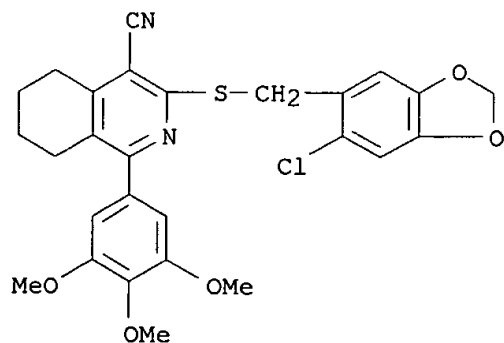
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 38 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 444156-75-6 REGISTRY  
 CN 3-Pyridinecarbonitrile, 6-(4-chlorophenyl)-2-[[[3,4-dichlorophenyl]methyl]thio]-4-(4-methylphenyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C26 H17 Cl3 N2 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

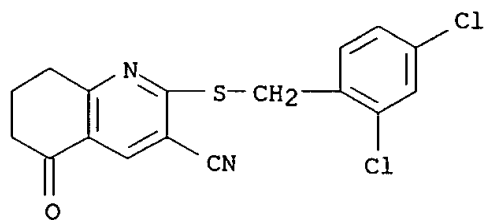
L4 ANSWER 39 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 444151-34-2 REGISTRY  
 CN 4-Isoquinolinecarbonitrile, 3-[[[6-chloro-1,3-benzodioxol-5-yl)methyl]thio]-5,6,7,8-tetrahydro-1-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C27 H25 Cl N2 O5 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

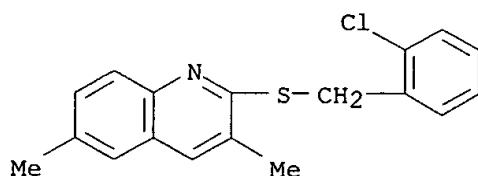
L4 ANSWER 40 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 444079-11-2 REGISTRY  
 CN 3-Quinolinecarbonitrile, 2-[[[(2,4-dichlorophenyl)methyl]thio]-5,6,7,8-tetrahydro-5-oxo- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C17 H12 Cl2 N2 O S  
 SR Chemical Library  
 LC STN Files: CHEMCATS





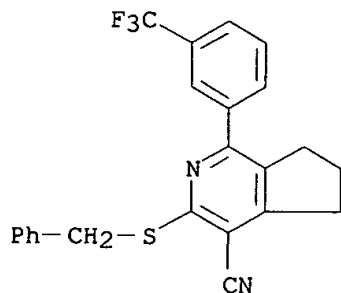
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 41 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 443745-43-5 REGISTRY  
 CN Quinoline, 2-[[2-chlorophenyl)methyl]thio]-3,6-dimethyl- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C18 H16 Cl N S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



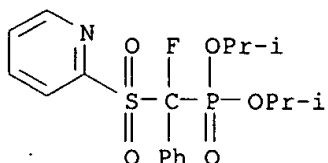
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 42 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 439108-57-3 REGISTRY  
 CN 5H-Cyclopenta[c]pyridine-4-carbonitrile, 6,7-dihydro-3-[(phenylmethyl)thio]-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C23 H17 F3 N2 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

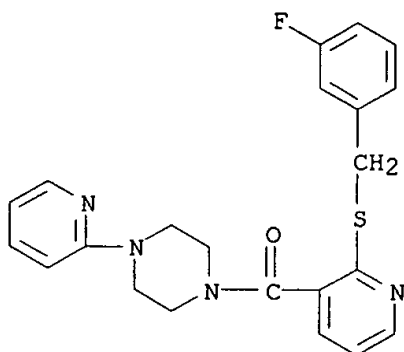
L4 ANSWER 43 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 428867-21-4 REGISTRY  
 CN Phosphonic acid, [fluorophenyl(2-pyridinylsulfonyl)methyl]-,  
 bis(1-methylethyl) ester (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN Diisopropyl [Fluoro(phenyl)(pyridin-2-ylsulfonyl)methyl]phosphonate  
 FS 3D CONCORD  
 MF C18 H23 F N O5 P S  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

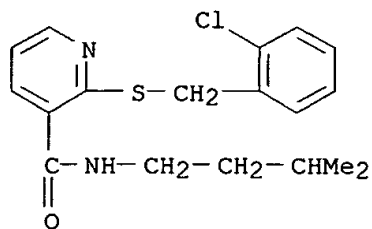
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 44 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 423146-99-0 REGISTRY  
 CN Piperazine, 1-[[2-[[[(3-fluorophenyl)methyl]thio]-3-pyridinyl]carbonyl]-4-(2-pyridinyl)]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C22 H21 F N4 O S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



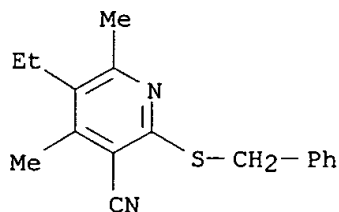
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 45 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 423146-88-7 REGISTRY  
 CN 3-Pyridinecarboxamide, 2-[[[(2-chlorophenyl)methyl]thio]-N-(3-methylbutyl)]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C18 H21 Cl N2 O S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



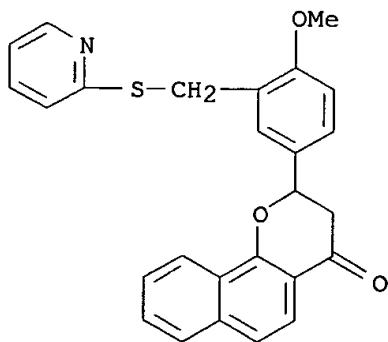
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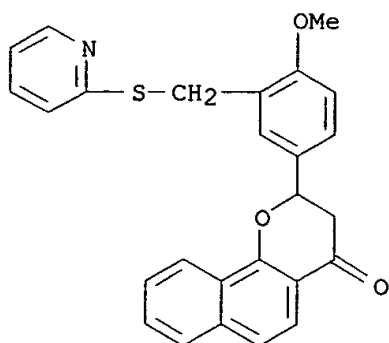
L4 ANSWER 46 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 413606-89-0 REGISTRY  
 CN 3-Pyridinecarbonitrile, 5-ethyl-4,6-dimethyl-2-[(phenylmethyl)thio]- (9CI)  
 (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C17 H18 N2 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

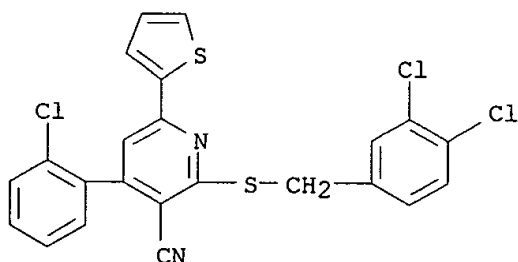
L4 ANSWER 47 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 404919-65-9 REGISTRY  
 CN 4H-Naphtho[1,2-b]pyran-4-one, 2,3-dihydro-2-[4-methoxy-3-[(2-pyridinylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C26 H21 N O3 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS





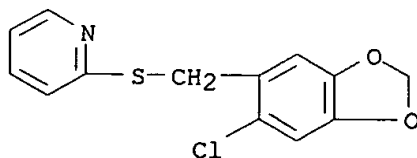
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 48 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 400737-74-8 REGISTRY  
 CN 3-Pyridinecarbonitrile, 4-(2-chlorophenyl)-2-[[3,4-dichlorophenyl)methyl]thio]-6-(2-thienyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C23 H13 Cl3 N2 S2  
 SR Chemical Library



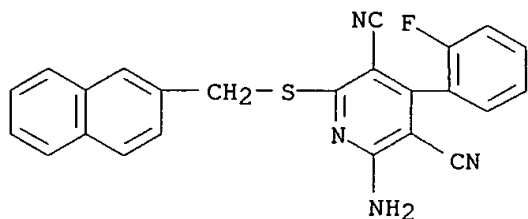
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 49 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 393126-92-6 REGISTRY  
 CN Pyridine, 2-[[6-chloro-1,3-benzodioxol-5-yl)methyl]thio]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C13 H10 Cl N O2 S  
 SR Chemical Library  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 50 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 391667-21-3 REGISTRY  
 CN 3,5-Pyridinedicarbonitrile, 2-amino-4-(2-fluorophenyl)-6-[(2-naphthalenylmethyl)thio]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C24 H15 F N4 S  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

93.96

94.17

FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004

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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4

FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 14

L5 10 L4

=> d 15 1-10

L5 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:133263 CAPLUS  
 DN 138:170241  
 TI Preparation of benzazepine derivatives as CCR5 antagonists  
 IN Shiraishi, Mitsuru; Baba, Masanori; Seto, Masaki; Aramaki, Yoshio;  
 Kanzaki, Naoyuki; Miyamoto, Naoki; Iizawa, Yuji  
 PA Takeda Chemical Industries, Ltd., Japan  
 SO PCT Int. Appl., 584 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003014110	A1	20030220	WO 2002-JP8045	20020807
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	JP 2003119191	A2	20030423	JP 2002-229553	20020807
PRAI	JP 2001-240718	A	20010808		
OS	MARPAT 138:170241				
RE.CNT	27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT				

L5 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:117800 CAPLUS  
 DN 138:153442  
 TI Preparation of heteroarylheteroalkylamines as inhibitors of nitric oxide  
 synthase  
 IN Birkinshaw, Timothy; Cheshire, David; Connolly, Stephen; Luker, Timothy;  
 Mete, Antonio  
 PA Astrazeneca AB, Swed.  
 SO PCT Int. Appl., 94 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003011830	A1	20030213	WO 2002-SE1413	20020726
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	SE 2001-2641	A	20010731		
OS	MARPAT 138:153442				
RE.CNT	6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD				

## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2002:974259 CAPLUS  
 DN 138:33310  
 TI Antiretroviral compounds and compositions  
 IN Brewer, Arthur D.; Cantor, Stephen E.; Dekeyser, Mark A.; Doweiko, Arthur  
 M. P.; Harris, John W.; Lacadie, John A.; Pierce, James B.; Mary, Louise  
 Jones Howard L.; Harrison, William A.  
 PA Uniroyal Chemical Company, Inc., USA  
 SO U.S., 19 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6498254	B1	20021224	US 2001-21202	20011029
	WO 2003037866	A1	20030508	WO 2002-US29573	20020917
	W: AU, BR, CA, CN, JP, MX				
PRAI	US 2001-21202	A	20011029		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2002:868910 CAPLUS  
 DN 137:352896  
 TI Preparation of arylheteroalkylamine derivatives as nitric oxide synthase  
 inhibitors useful as anti-inflammatories and analgesics  
 IN Birkinshaw, Tim; Connolly, Stephen; Luker, Timothy; Mete, Antonio;  
 Millichip, Ian  
 PA Astrazeneca AB, Swed.  
 SO PCT Int. Appl., 123 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002090332	A2	20021114	WO 2002-SE876	20020506
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI SE 2001-1617 A 20010508  
 SE 2001-3271 A 20010928  
 OS MARPAT 137:352896

L5 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2002:834242 CAPLUS  
 DN 139:26483  
 TI Lipophilicity characterization by reversed-phase HPLC of potential  
 antituberculosics  
 AU Kastner, Petr; Klimes, Jiri; Velenovska, Petra; Klimesova, Vera  
 CS Faculty of Pharmacy in Hradec Kralove, Charles University in Prague,  
 Hradec Kralove, 500 05, Czech Rep.

SO Journal of Liquid Chromatography & Related Technologies (2002), 25(18),  
2849-2856  
CODEN: JLCTFC; ISSN: 1082-6076  
PB Marcel Dekker, Inc.  
DT Journal  
LA English  
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:805644 CAPLUS  
DN 138:201546  
TI Pyridine oxide derivatives: Structure-activity relationship for inhibition  
of human immunodeficiency virus and cytomegalovirus replication in cell  
culture  
AU Balzarini, Jan; Stevens, Miguel; Andrei, Graciela; Snoeck, Robert; Strunk,  
Richard; Pierce, James B.; Lacadie, John A.; De Clercq, Erik; Pannecouque,  
Christophe  
CS Rega Institute for Medical Research, Katholieke Universiteit Leuven,  
Louvain, B-3000, Belg.  
SO Helvetica Chimica Acta (2002), 85(9), 2961-2975  
CODEN: HCACAV; ISSN: 0018-019X  
PB Verlag Helvetica Chimica Acta  
DT Journal  
LA English  
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:695954 CAPLUS  
DN 137:216880  
TI Preparation of 2-thio-3,5-dicyano-4-aryl-6-aminopyridines as adenosine  
receptor-selective ligands  
IN Rosentreter, Ulrich; Kraemer, Thomas; Vaupe, Andrea; Huebsch, Walter;  
Diedrichs, Nicole; Krahn, Thomas; Dembowski, Klaus; Stasch, Johannes-Peter  
PA Bayer Aktiengesellschaft, Germany  
SO PCT Int. Appl., 69 pp.  
CODEN: PIXXD2  
DT Patent  
LA German  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002070485	A1	20020912	WO 2002-EP2121	20020228
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
	CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				
	GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				
	LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,				
	PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,				
	UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,				
	TJ, TM				
	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,				
	CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,				
	BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 10110754	A1	20020919	DE 2001-10110754	20010307
	EP 1368319	A1	20031210	EP 2002-702377	20020228
	R:				
	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
	IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	DE 2001-10110754	A	20010307		
	WO 2002-EP2121	W	20020228		
OS	MARPAT 137:216880				
RE.CNT	4				
	THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD				



## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:695053 CAPLUS  
DN 138:153519  
TI Tributylphosphine-catalyzed acylation of alcohol by active ester directed toward effective end-capping of pseudorotaxane consisting of ammonium group and crown ether  
AU Kihara, Nobuhiro; Nakakoji, Naohisa; Takata, Toshikazu  
CS Department of Applied Chemistry, Graduate School of Engineering, Osaka Prefecture University, Osaka, 599-8531, Japan  
SO Chemistry Letters (2002), (9), 924-925  
CODEN: CMLTAG; ISSN: 0366-7022  
PB Chemical Society of Japan  
DT Journal  
LA English  
OS CASREACT 138:153519  
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:229584 CAPLUS  
DN 136:401835  
TI Studies toward the Synthesis of .alpha.-Fluorinated Phosphonates via Tin-Mediated Cleavage of .alpha.-Fluoro-.alpha.-(pyrimidin-2-ylsulfonyl)alkylphosphonates. Intramolecular Cyclization of the .alpha.-Phosphonyl Radicals  
AU Wnuk, Stanislaw F.; Bergolla, Luis A.; Garcia, Pedro I., Jr.  
CS Department of Chemistry, Florida International University, Miami, FL, 33199, USA  
SO Journal of Organic Chemistry (2002), 67(9), 3065-3071  
CODEN: JOCEAH; ISSN: 0022-3263  
PB American Chemical Society  
DT Journal  
LA English  
OS CASREACT 136:401835  
RE.CNT 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:72052 CAPLUS  
DN 136:118474  
TI Preparation of dicyanopyridine derivatives as high-conductance calcium-sensitive potassium channel openers  
IN Harada, Hironori; Watanuki, Susumu; Takuwa, Tomofumi; Kawaguchi, Kenichi; Okazaki, Toshio; Hirano, Yuusuke; Saitoh, Chikashi  
PA Yamanouchi Pharmaceutical Co., Ltd., Japan  
SO PCT Int. Appl., 92 pp.  
CODEN: PIXXD2  
DT Patent  
LA Japanese  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	WO 2002006237	A1	20020124	WO 2001-JP6136	20010716
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,			

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 AU 2001069529 A5 20020130 AU 2001-69529 20010716  
 EP 1302463 A1 20030416 EP 2001-948028 20010716  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 US 2003232860 A1 20031218 US 2003-333264 20030117  
 PRAI JP 2000-216982 A 20000718  
 WO 2001-JP6136 W 20010716  
 OS MARPAT 136:118474  
 RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L5 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2002:974259 CAPLUS  
 DN 138:33310  
 ED Entered STN: 26 Dec 2002  
 TI Antiretroviral compounds and compositions  
 IN Brewer, Arthur D.; Cantor, Stephen E.; Dekeyser, Mark A.; Doweiko, Arthur  
 M. P.; Harris, John W.; Lacadie, John A.; Pierce, James B.; Mary, Louise  
 Jones Howard L.; Harrison, William A.  
 PA Uniroyal Chemical Company, Inc., USA  
 SO U.S., 19 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A61K031-47  
 ICS C07D215-16; C07D211-72; C07D211-84  
 NCL 546157000; 546290000; 546294000; 514312000; 514345000; 514347000  
 CC 1-5 (Pharmacology)  
 Section cross-reference(s): 27  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6498254	B1	20021224	US 2001-21202	20011029
	WO 2003037866	A1	20030508	WO 2002-US29573	20020917
	W: AU, BR, CA, CN, JP, MX				
PRAI	US 2001-21202	A	20011029		

AB Certain pyridine and quinoline derivs. which inhibit replication of the  
 retroviruses HIV-1, HIV-2 and human cytomegalovirus (HCMV) are provided.  
 Pharmaceutical compns. useful in methods of treating or inhibiting certain  
 retrovirus infections are described.  
 ST antiretroviral compd pyridine quinoline deriv  
 IT Anti-AIDS agents  
 Antiviral agents  
 Human  
 Human herpesvirus 5  
 Human immunodeficiency virus 1  
 Human immunodeficiency virus 2  
 (antiretroviral compds. and compns. using pyridine and quinoline  
 derivs.)  
 IT Drug delivery systems  
 (carriers; antiretroviral compds. and compns. using pyridine and  
 quinoline derivs.)  
 IT 478620-19-8P 478620-24-5P 478620-25-6P 478620-28-9P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic  
 preparation); THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (antiretroviral compds. and compns. using pyridine and quinoline

derivs.)

IT 69212-31-3P, 2-Benzylthio-3-nitropyridine 478619-45-3P 478619-49-7P  
 478619-53-3P 478619-57-7P 478619-61-3P 478619-65-7P 478619-68-0P  
 478619-72-6P 478619-78-2P 478619-82-8P 478619-86-2P 478619-90-8P  
 478619-94-2P 478619-98-6P 478620-02-9P 478620-06-3P 478620-08-5P  
 478620-11-0P 478620-12-1P 478620-14-3P 478620-16-5P 478620-18-7P  
 478620-20-1P 478620-21-2P 478620-23-4P 478620-26-7P 478620-27-8P  
 478620-29-0P 478620-30-3P 478620-31-4P 478620-32-5P 478620-33-6P  
 478620-34-7P 478620-35-8P 478620-36-9P 478620-37-0P 478620-38-1P  
 478620-39-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(antiretroviral compds. and compns. using pyridine and quinoline  
 derivs.)

IT 51-79-6, Urethane 86-81-7, 3,4,5-Trimethoxybenzaldehyde 100-44-7,  
 Benzyl chloride, reactions 100-52-7, Benzaldehyde, reactions 100-53-8,  
 Benzylmercaptan 123-11-5, 4-Methoxybenzaldehyde, reactions 607-66-9,  
 2-Hydroxy-4-methylquinoline 824-45-3, 2,5-Dimethylbenzyl chloride  
 2014-83-7, 2,6-Dichlorobenzyl chloride 2044-27-1, 1-Methyl-2(1H)-  
 pyridinethione 2587-00-0, 2,6-Dichloropyridine-N-oxide 2637-34-5,  
 2-Mercaptopyridine 3811-73-2 5470-18-8, 2-Chloro-3-nitropyridine  
 6258-60-2, 4-Methoxybenzylmercaptan 20871-93-6 22182-98-5  
 52694-50-5, 3-Chloromethyl-1-methylpiperidine 53976-62-8 53976-65-1  
 60263-88-9 82959-54-4 84504-48-3 91668-83-6, 2-Chloro-3-  
 methylpyridine-N-oxide 338778-95-3 478619-47-5 478619-51-1  
**478619-55-5** 478619-59-9 478619-63-5 478619-70-4  
 478619-76-0 478619-80-6 478619-84-0 478619-88-4 478619-92-0  
 478619-96-4 478620-00-7 478620-05-2 478620-07-4 478620-09-6  
 478620-10-9 478620-13-2 478620-15-4 478620-17-6 478620-22-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(antiretroviral compds. and compns. using pyridine and quinoline  
 derivs.)

IT 4437-65-4P 81167-65-9P 81167-66-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(antiretroviral compds. and compns. using pyridine and quinoline  
 derivs.)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Brouwer; US 5696151 A 1997 CAPLUS  
 (2) Harrison; US 5268389 A 1993 CAPLUS  
 (3) Moormann; US 5945425 A 1999 CAPLUS

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(FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004

L1 STRUCTURE UPLOADED  
 L2 0 S L1 EXA SAM  
 L3 0 S L1 FAM SAM  
 L4 50 S L1 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004

L5 10 S L4

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

16.53

110.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	-0.69	-0.69

FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4  
DICTIONARY FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d his

(FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004

L1 STRUCTURE UPLOADED  
L2 0 S L1 EXA SAM  
L3 0 S L1 FAM SAM  
L4 50 S L1 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004

L5 10 S L4

FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004

=> s l1 sss full

FULL SEARCH INITIATED 09:32:29 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 11171 TO ITERATE

100.0% PROCESSED 11171 ITERATIONS 4073 ANSWERS  
SEARCH TIME: 00.00.01

L6 4073 SEA SSS FUL L1

=> s hiv or retroviral or retrovirus

653 HIV  
162 RETROVIRAL  
2918 RETROVIRUS  
L7 3719 HIV OR RETROVIRAL OR RETROVIRUS

=> s herpes or herpetic or hsv or hcmv or cmv or hhv

2328 HERPES  
0 HERPETIC  
26 HSV

7 HCMV  
62 CMV  
0 HHV  
L8 2422 HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	196.55	307.25

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.69

FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4  
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s hiv or retroviral or retrovirus

52913 HIV  
14315 RETROVIRAL  
11976 RETROVIRUS

L9 70667 HIV OR RETROVIRAL OR RETROVIRUS

=> s herpes or herpetic or hsv or hcmv or cmv or hhv

22109 HERPES  
849 HERPETIC  
9988 HSV  
2423 HCMV  
5770 CMV  
1166 HHV

L10 31317 HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

=> d his

(FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004

L1 STRUCTURE UPLOADED  
L2 0 S L1 EXA SAM  
L3 0 S L1 FAM SAM  
L4 50 S L1 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004  
L5 10 S L4

FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004  
L6 4073 S L1 SSS FULL  
L7 3719 S HIV OR RETROVIRAL OR RETROVIRUS  
L8 2422 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004  
L9 70667 S HIV OR RETROVIRAL OR RETROVIRUS  
L10 31317 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

=> s 16

L11 636 L6

=> s 111 and 19

L12 9 L11 AND L9

=> d 112 1-9

L12 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:356233 CAPLUS

DN 138:368768

TI Method for treating human immunodeficiency virus (HIV),  
cytomegalovirus, (HCMV), and herpes virus (HHV) **retroviral**  
infections by administration of heteroarenes.

IN Lacadie, John A.; Pierce, James

PA Uniroyal Chemical Company, Inc., USA

SO PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003037311	A2	20030508	WO 2002-US31836	20021003
	WO 2003037311	A3	20031016		
	W: AU, BR, CA, CN, JP, MX				
	US 2003139445	A1	20030724	US 2001-21453	20011029
PRAI	US 2001-21453	A	20011029		
OS	MARPAT 138:368768				

L12 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:974259 CAPLUS

DN 138:33310

TI Antiretroviral compounds and compositions

IN Brewer, Arthur D.; Cantor, Stephen E.; Dekeyser, Mark A.; Dowejko, Arthur  
M. P.; Harris, John W.; Lacadie, John A.; Pierce, James B.; Mary, Louise  
Jones Howard L.; Harrison, William A.

PA Uniroyal Chemical Company, Inc., USA

SO U.S., 19 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6498254	B1	20021224	US 2001-21202	20011029
	WO 2003037866	A1	20030508	WO 2002-US29573	20020917
	W: AU, BR, CA, CN, JP, MX				
PRAI	US 2001-21202	A	20011029		
RE.CNT	3				

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:805644 CAPLUS  
DN 138:201546  
TI Pyridine oxide derivatives: Structure-activity relationship for inhibition of human immunodeficiency virus and cytomegalovirus replication in cell culture  
AU Balzarini, Jan; Stevens, Miguel; Andrei, Graciela; Snoeck, Robert; Strunk, Richard; Pierce, James B.; Lacadie, John A.; De Clercq, Erik; Pannecouque, Christophe  
CS Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.  
SO Helvetica Chimica Acta (2002), 85(9), 2961-2975  
CODEN: HCACAV; ISSN: 0018-019X  
PB Verlag Helvetica Chimica Acta  
DT Journal  
LA English  
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:695955 CAPLUS  
DN 137:232650  
TI Preparation of nitrogen-containing heteroaryl compounds having HIV integrase inhibitory activity  
IN Fuji, Masahiro; Mikamiyama, Hidenori; Murai, Hitoshi  
PA Shionogi & Co., Ltd., Japan  
SO PCT Int. Appl., 316 pp.  
CODEN: PIXXD2  
DT Patent  
LA Japanese  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002070486	A1	20020912	WO 2002-JP1778	20020227
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	EP 1375486	A1	20040102	EP 2002-701583	20020227
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
PRAI	JP 2001-57037	A	20010301		
	JP 2001-243530	A	20010810		
	JP 2001-395022	A	20011226		
	WO 2002-JP1778	W	20020227		
OS	MARPAT 137:232650				

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2000:784381 CAPLUS  
DN 133:335153  
TI Preparation of N-arylmethylthioanilide compounds useful for the inhibition of the replication of HIV  
IN Brouwer, Walter Gerhard; Osika, Ewa Maria

PA Uniroyal Chemical Co., Inc., USA; Uniroyal Chemical Co./cie.  
SO U.S., 9 pp.  
CODEN: USXXAM  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6143780	A	20001107	US 1999-398649	19990917
	WO 2001019811	A2	20010322	WO 2000-US24986	20000912
	WO 2001019811	A3	20010726		
	W: CA				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 1220848	A2	20020710	EP 2000-963380	20000912
	EP 1220848	B1	20031119		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
	AT 254611	E	20031215	AT 2000-963380	20000912
PRAI	US 1999-398649	A	19990917		
	WO 2000-US24986	W	20000912		
OS	MARPAT 133:335153				

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1999:705001 CAPLUS  
DN 131:322530  
TI Substituted tetronic acids useful for treating HIV and other retroviruses  
IN Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin, James M.; Smith, Clark W.; Tommasi, Ruben A.; Aristoff, Paul A.; Skulnick, Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.  
PA USA  
SO U.S., 116 pp., Cont.-in-part of U.S. Ser. No. 238,820, abandoned.  
CODEN: USXXAM

DT Patent  
LA English  
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5977169	A	19991102	US 1997-604937	19970728
	ZA 9406099	A	19960212	ZA 1994-6099	19940812
	WO 9507901	A1	19950323	WO 1994-US9533	19940907
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
	RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
PRAI	US 1993-123029		19930917		
	US 1994-238820		19940506		
	WO 1994-US9533		19940907		
OS	MARPAT 131:322530				

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1999:585082 CAPLUS  
DN 131:331727  
TI Structure Based Prediction of Binding Affinity of Human Immunodeficiency Virus-1 Protease Inhibitors



AU Kulkarni, Santosh S.; Kulkarni, Vithal M.  
 CS Pharmaceutical Division Department of Chemical Technology, University of  
 Mumbai, Matunga Mumbai, 400 019, India  
 SO Journal of Chemical Information and Computer Sciences (1999), 39(6),  
 1128-1140  
 CODEN: JCISD8; ISSN: 0095-2338  
 PB American Chemical Society  
 DT Journal  
 LA English  
 RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1997:165733 CAPLUS  
 DN 126:258470  
 TI Synthesis and pharmacological evaluation of sulfone substituted  
 HIV protease inhibitors  
 AU Schwartz, Theresa M.; Bundy, Gordon L.; Strohbach, Joseph W.;  
 Thairrivongs, Suvit; Johnson, Paul D.; Skulnick, Harvey I.; Tomich, Paul  
 K.; Lynn, Janet C.; Chong, Kong Teck; Hinshaw, Roger R.; Raub, Thomas J.;  
 Padbury, Guy E.; Loth, Lisa N.  
 CS Res. Labs., Pharmacia Upjohn, Inc., Kalamazoo, MI, 49001-0199, USA  
 SO Bioorganic & Medicinal Chemistry Letters (1997), 7(4), 399-402  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PB Elsevier  
 DT Journal  
 LA English  
 RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1995:648144 CAPLUS  
 DN 123:55683  
 TI Substituted tetronic acids useful for treating HIV and other  
 retroviruses  
 IN Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin,  
 James M.; Smith, Clark W.; Tommasi, Rubin A.; Aristoff, Paul A.; Skulnick,  
 Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.  
 PA Upjohn Co., USA  
 SO PCT Int. Appl., 223 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9507901	A1	19950323	WO 1994-US9533	19940907
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
	RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	ZA 9406099	A	19960212	ZA 1994-6099	19940812
	CA 2168757	AA	19950323	CA 1994-2168757	19940907
	AU 9476368	A1	19950403	AU 1994-76368	19940907
	EP 720607	A1	19960710	EP 1994-926571	19940907
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 09502713	T2	19970318	JP 1994-509195	19940907
	US 5977169	A	19991102	US 1997-604937	19970728
PRAI	US 1993-123029		19930917		
	US 1994-238820		19940506		

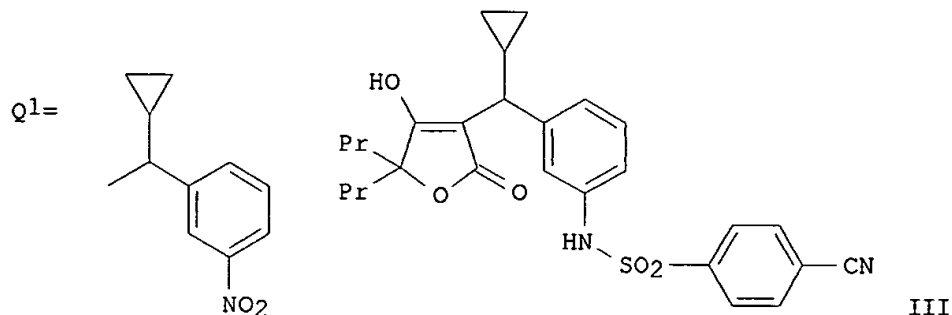
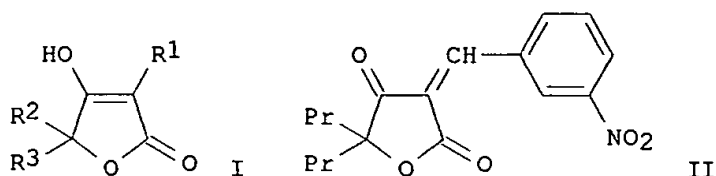
WO 1994-US9533 19940907  
OS MARPAT 123:55683

=> d 112 9 all

L12 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1995:648144 CAPLUS  
DN 123:55683  
ED Entered STN: 01 Jul 1995  
TI Substituted tetronic acids useful for treating HIV and other  
retroviruses  
IN Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin,  
James M.; Smith, Clark W.; Tommasi, Rubin A.; Aristoff, Paul A.; Skulnick,  
Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.  
PA Upjohn Co., USA  
SO PCT Int. Appl., 223 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
IC ICM C07D307-60  
ICS A61K031-365; C07D307-94; C07D405-06; C07D405-12; C07D491-10  
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 1

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9507901	A1	19950323	WO 1994-US9533	19940907
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
	RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	ZA 9406099	A	19960212	ZA 1994-6099	19940812
	CA 2168757	AA	19950323	CA 1994-2168757	19940907
	AU 9476368	A1	19950403	AU 1994-76368	19940907
	EP 720607	A1	19960710	EP 1994-926571	19940907
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 09502713	T2	19970318	JP 1994-509195	19940907
	US 5977169	A	19991102	US 1997-604937	19970728
PRAI	US 1993-123029		19930917		
	US 1994-238820		19940506		
	WO 1994-US9533		19940907		
OS	MARPAT 123:55683				
GI					



AB The invention comprises novel substituted tetronic acid derivs. I and tautomers [wherein R1-R3 = wide variety of specified C-contg. substituents]. I are inhibitors of **HIV** protease, and may be useful for treatment of AIDS or AIDS-related diseases. I may also be used to retard replication of any **retrovirus** contg. aspartyl protease. Approx. 250 compds. are claimed, and phys. and biol. data for approx. 115 compds. are provided. For example, condensation of I [R1 = H, R2 = R3 = Pr] with 3-nitrobenzaldehyde gave >100% crude nitrobenzylidene deriv. II, which reacted with cyclopropylmagnesium bromide and CuBr.SMe<sub>2</sub> in THF to give 62% I [R1 = Q1, R2 = R3 = Pr]. Hydrogenation of the nitro group (97%) and sulfonamidation of the resultant amino group with 4-cyanobenzenesulfonyl chloride (53%) gave title compd. III, a preferred compd. Several compds. including III are said to have inhibited replication of **HIV-1** in human cell lines. **HIV-1** protease inhibitory data are provided.

ST tetronic acid prepn antiviral **retrovirus**; furandione prepn antiviral **retrovirus**; **HIV** protease inhibitor tetronic acid prepn

IT Virucides and Virustats  
(prepn. of antiretroviral tetronic acid derivs.)

IT Acquired immune deficiency syndrome  
(treatment; prepn. of antiretroviral tetronic acid derivs.)

IT Virus, animal  
(human immunodeficiency, inhibition; prepn. of antiretroviral tetronic acid derivs.)

IT Virus, animal  
(human immunodeficiency 1, inhibition; prepn. of antiretroviral tetronic acid derivs.)

IT 144114-21-6, Retropepsin  
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)  
(inhibitors of **HIV**; prepn. of antiretroviral tetronic acid derivs.)

IT 78169-47-8, Aspartyl protease  
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)  
(inhibitors; prepn. of antiretroviral tetronic acid derivs.)

IT 1138-44-9P 10424-93-8P 72036-34-1P 85520-35-0P 129042-95-1P  
161720-04-3P 164344-89-2P 164344-98-3P 164345-52-2P 164346-90-1P  
164346-91-2P 164346-92-3P 164346-93-4P 164346-94-5P 164346-95-6P

164346-96-7P	164346-98-9P	164346-99-0P	164347-00-6P	164347-01-7P
164347-02-8P	164347-03-9P	164347-04-0P	164347-07-3P	164347-08-4P
164347-09-5P	164347-10-8P			

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of antiretroviral tetronic acid derivs.)

IT	164344-46-1P	164344-47-2P	164344-48-3P	164344-49-4P	164344-50-7P
	164344-51-8P	164344-52-9P	164344-53-0P	164344-54-1P	164344-55-2P
	164344-56-3P	164344-57-4P	164344-58-5P	164344-59-6P	164344-60-9P
	164344-61-0P	164344-62-1P	164344-63-2P	164344-64-3P	164344-65-4P
	164344-66-5P	164344-67-6P	164344-68-7P	164344-69-8P	164344-70-1P
	164344-71-2P	164344-72-3P	164344-73-4P	164344-74-5P	164344-75-6P
	164344-76-7P	164344-77-8P	164344-78-9P	164344-79-0P	164344-80-3P
	164344-81-4P	164344-82-5P	164344-83-6P	164344-84-7P	164344-85-8P
	164344-86-9P	164344-87-0P	164344-88-1P	164344-89-2P	164344-90-5P
	164344-91-6P	164344-92-7P	164344-93-8P	164344-94-9P	164344-95-0P
	164344-96-1P	164344-97-2P	164344-98-3P	164344-99-4P	164345-00-0P
	164345-01-1P	164345-02-2P	164345-03-3P	164345-04-4P	164345-05-5P
	164345-06-6P	164345-07-7P	164345-08-8P	164345-09-9P	164345-10-2P
	164345-11-3P	164345-12-4P	164345-13-5P	164345-14-6P	164345-15-7P
	164345-16-8P	164345-17-9P	164345-18-0P	164345-19-1P	164345-20-4P
	164345-21-5P	164345-22-6P	164345-23-7P	164345-24-8P	164345-25-9P
	164345-26-0P	164345-27-1P	164345-28-2P	164345-29-3P	164345-30-6P
	164345-31-7P	164345-32-8P	164345-33-9P	164345-34-0P	164345-35-1P
	164345-36-2P	164345-37-3P	164345-38-4P	164345-39-5P	164345-40-8P
	164345-41-9P	164345-42-0P	164345-43-1P	164345-44-2P	164345-45-3P
	164345-46-4P	164345-47-5P	164345-48-6P	164345-49-7P	164345-50-0P
	164345-51-1P	164345-52-2P	164345-53-3P	164345-54-4P	164345-55-5P
	164345-56-6P	164345-58-8P	164345-59-9P	164345-60-2P	164345-61-3P
	164345-62-4P	164345-63-5P	164345-64-6P	164345-65-7P	164345-66-8P
	164345-67-9P	164345-68-0P	164345-69-1P	164345-70-4P	164345-71-5P
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	164345-82-8P	164345-83-9P	164345-84-0P	164345-85-1P	164345-86-2P
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	<b>164346-46-7P</b>	<b>164346-47-8P</b>	164346-48-9P	164346-49-0P	
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	<b>164346-71-8P</b>	164346-72-9P	164346-73-0P	164346-74-1P	
	164346-75-2P	164346-76-3P	164346-77-4P	164346-78-5P	164346-79-6P
	164346-80-9P				

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of antiretroviral tetronic acid derivs.)

IT	<b>164346-81-0P</b>	<b>164346-82-1P</b>	<b>164346-83-2P</b>		
	164346-84-3P	164346-85-4P	164346-86-5P	164346-87-6P	164346-88-7P
	164346-89-8P				

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of antiretroviral tetronic acid derivs.)

IT 57-14-7, 1,1-Dimethylhydrazine 74-96-4, Bromoethane 99-61-6,  
3-Nitrobenzaldehyde 100-39-0, Benzyl bromide 103-63-9,  
(2-Bromoethyl)benzene 104-53-0, Hydrocinnamaldehyde 106-94-5, Propyl  
bromide 108-94-1, Cyclohexanone, reactions 120-92-3, Cyclopentanone  
123-19-3, 4-Heptanone 501-53-1, Benzyl chloroformate 502-49-8,  
Cyclooctanone 623-47-2, Ethyl propiolate 637-59-2,  
1-Bromo-3-phenylpropane 946-33-8, 2-Benzylcyclohexanone 1007-03-0,  
.alpha.-Cyclopropylbenzyl alcohol 1067-74-9, Methyl  
diethylphosphonoacetate 1138-44-9 2550-26-7, Benzyl acetone  
2637-37-8, 2-Quinolinethiol 4423-94-3, 2-Ethylcyclohexanone 4971-56-6,  
Tetronic acid 14371-10-9, trans-Cinnamaldehyde 23719-80-4,  
Cyclopropylmagnesium bromide 28920-43-6, 9-Fluorenylmethyl chloroformate  
29976-53-2, 1-Carbethoxy-4-piperidone 49584-26-1, 4-Cyanobenzenesulfonyl  
chloride 118753-70-1 164345-06-6 164346-97-8 164347-05-1  
164347-06-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; prepn. of antiretroviral tetronic acid derivs.)

=> d 112 8 all

L12 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:165733 CAPLUS

DN 126:258470

ED Entered STN: 12 Mar 1997

TI Synthesis and pharmacological evaluation of sulfone substituted  
HIV protease inhibitors

AU Schwartz, Theresa M.; Bundy, Gordon L.; Strohbach, Joseph W.;  
Thairrivongs, Suvit; Johnson, Paul D.; Skulnick, Harvey I.; Tomich, Paul  
K.; Lynn, Janet C.; Chong, Kong Teck; Hinshaw, Roger R.; Raub, Thomas J.;  
Padbury, Guy E.; Loth, Lisa N.

CS Res. Labs., Pharmacia Upjohn, Inc., Kalamazoo, MI, 49001-0199, USA

SO Bioorganic & Medicinal Chemistry Letters (1997), 7(4), 399-402

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier

DT Journal

LA English

CC 1-3 (Pharmacology)

AB The sulfonamide substituted pyranones (1) have recently been shown to be  
potent HIV protease inhibitors. We prepared a series of sulfone  
substituted analogs and compared and their biol. activities to those of  
the corresponding sulfonamide analogs. It was detd. that although these  
comps. maintained activity as enzyme inhibitors, they showed somewhat  
diminished antiviral activity event though they may possess increased  
membrane permeability.

ST sulfonamide pyranone prepn HIV protease inhibitor

IT Structure-activity relationship

(antiviral; sulfonamide substituted pyranones as HIV protease  
inhibitors)

IT Structure-activity relationship

(aspartic proteinase-inhibiting; sulfonamide substituted pyranones as  
HIV protease inhibitors)

IT Anti-AIDS agents

Antiviral agents

Human immunodeficiency virus 1

(sulfonamide substituted pyranones as HIV protease  
inhibitors)

IT 174483-90-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(antiviral and HIV-1 protease inhibiting activity of)

IT 166335-18-8P 166335-24-6P 166335-32-6P 166335-74-6P 166335-80-4P  
174483-25-1P 174483-26-2P 174483-27-3P 174483-28-4P 174483-29-5P  
174483-30-8P 174483-56-8P 174483-62-6P 174483-63-7P 174483-94-4P  
**188839-13-6P 188839-14-7P 188839-15-8P 188839-16-9P**  
188839-17-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and antiviral and HIV-1 protease inhibiting activity of)

IT 162174-73-4P 174484-94-7P 188839-19-2P 188839-20-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of)

IT 675-10-5 7051-34-5, Bromomethyl cyclopropane 100058-82-0 174484-93-6  
188839-18-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of)

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

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=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	36.86	344.11
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.39	-2.08

FILE 'REGISTRY' ENTERED AT 09:41:14 ON 21 JAN 2004

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DICTIONARY FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> S 188839-16-9/RN

L13 1 188839-16-9/RN

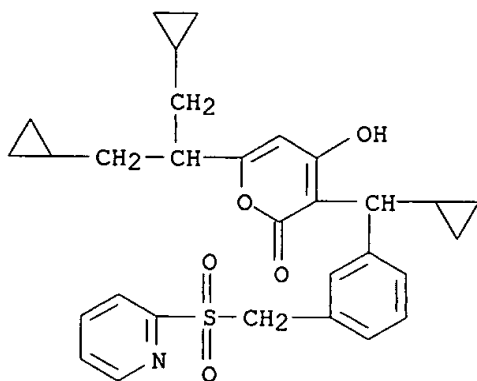
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NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> D L13 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y  
THE ESTIMATED COST FOR THIS REQUEST IS 5.92 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 188839-16-9 REGISTRY  
CN 2H-Pyran-2-one, 6-[2-cyclopropyl-1-(cyclopropylmethyl)ethyl]-3-  
[cyclopropyl[3-[(2-pyridinylsulfonyl)methyl]phenyl]methyl]-4-hydroxy-  
(9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C30 H33 N O5 S  
SR CA  
LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=>

=> d 112 7 all

YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:n

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.61	346.72
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.08

FILE 'CAPLUS' ENTERED AT 09:42:34 ON 21 JAN 2004  
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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4  
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 112 7 all

L12 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1999:585082 CAPLUS  
DN 131:331727  
ED Entered STN: 20 Sep 1999  
TI Structure Based Prediction of Binding Affinity of Human Immunodeficiency Virus-1 Protease Inhibitors  
AU Kulkarni, Santosh S.; Kulkarni, Vithal M.  
CS Pharmaceutical Division Department of Chemical Technology, University of Mumbai, Matunga Mumbai, 400 019, India  
SO Journal of Chemical Information and Computer Sciences (1999), 39(6), 1128-1140  
CODEN: JCISD8; ISSN: 0095-2338  
PB American Chemical Society  
DT Journal  
LA English  
CC 1-3 (Pharmacology)  
Section cross-reference(s): 7, 22  
AB A series of computations were performed to derive a strategy for the prediction of binding affinities of non-peptidic human immunodeficiency virus-1 (HIV-1) protease inhibitors. This paper describes the development of a 3D quant. structure-activity relation (3D-QSAR) methodol. by using receptor information of HIV-1 protease. The docking and mol. dynamics simulations were performed on a model ligand/enzyme complex to optimize the variables involved in the generation of



ligand/enzyme models. The protonation scheme of the active site aspartic acid residues of HIV-1 protease was derived from a computational study. The active site aspartate is monoprotonated with a proton placed on the OD1 atom of the ASP B25. This protocol of docking and mol. dynamics (MD) simulation was then used to derive the ligand-enzyme complexes of the mols. used in the present study. The mol. mechanics interaction descriptors were calcd. from these ligand/enzyme models. A partial least squares (PLS) method was used to derive a linear correlation between the interaction descriptors and the biol. activity. A good correlation was obsd. when the change in the energy of the ligand upon complex formation and the electrostatic contributions to the solvation energy of the ligand were included in the QSAR anal. A highest cross-validated q<sup>2</sup> value of 0.649 was obsd. This model had a conventional r<sup>2</sup> of 0.725, and when this model was used to predict the activity of the external test set, it produced a r<sup>2</sup>pred of 0.761. The total interaction energy was partitioned into interactions in different subsites and interactions with each of the amino acid residues of the enzyme. The PLS anal. using these descriptors helped to identify the important interactions which can be exploited for the design of HIV-1 protease inhibitors.

ST HIV1 virus protease inhibitor QSAR design; drug design HIV1 virus protease inhibitor

IT Enzyme functional sites

(active; structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

IT Simulation and Modeling, biological

(mol. dynamics; structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

IT Conformation

Human immunodeficiency virus 1

Molecular association

Molecular modeling

Potential energy

QSAR (structure-activity relationship)

(structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

IT 81-81-2 435-97-2 149394-65-0 158200-29-4 162168-60-7 162168-64-1  
 162168-92-5 162169-60-0 162169-80-4 162169-86-0 163020-86-8  
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 174484-54-9 176771-70-3 183963-05-5 183964-16-1 **188839-16-9**  
 188839-17-0 213014-48-3 249765-76-2 249765-77-3

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

IT 144114-21-6, Retropepsin

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)

(structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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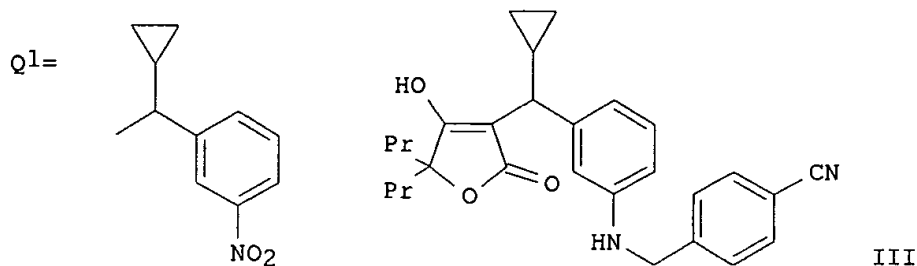
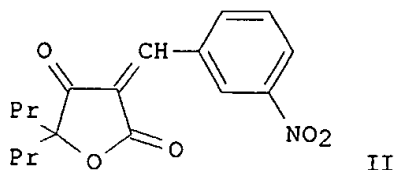
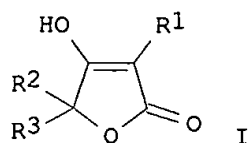
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=> d 112 6 all

L12 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1999:705001 CAPLUS  
 DN 131:322530  
 ED Entered STN: 04 Nov 1999  
 TI Substituted tetronic acids useful for treating HIV and other  
 retroviruses  
 IN Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin,  
 James M.; Smith, Clark W.; Tommasi, Ruben A.; Aristoff, Paul A.; Skulnick,  
 Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.  
 PA USA  
 SO U.S., 116 pp., Cont.-in-part of U.S. Ser. No. 238,820, abandoned.  
 CODEN: USXXAM

DT Patent  
 LA English  
 IC ICM A61K031-34  
 ICS A61K031-335; A61K031-415; A61K031-505  
 NCL 514473000  
 CC 27-6 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 1  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5977169	A	19991102	US 1997-604937	19970728
	ZA 9406099	A	19960212	ZA 1994-6099	19940812
	WO 9507901	A1	19950323	WO 1994-US9533	19940907
	W:				AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN
	RW:				KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
PRAI	US 1993-123029		19930917		
	US 1994-238820		19940506		
	WO 1994-US9533		19940907		
OS	MARPAT 131:322530				
GI					



AB The invention comprises novel substituted tetronic acid derivs. (I) and tautomers [wherein R1-R3 = wide variety of specified C-contg. substituents] that are inhibitors of HIV protease. I retard replication of any **retrovirus** contg. aspartyl protease and are useful for treatment of AIDS or AIDS-related diseases. Approx. 250 compds. are claimed, and phys. and biol. data for approx. 120 compds. are provided. For example, condensation of I [R1 = H, R2 = R3 = Pr] with 3-nitrobenzaldehyde gave >100% crude nitrobenzylidene deriv. II, which reacted with cyclopropylmagnesium bromide and CuBr.SMe2 in THF to give 62% I [R1 = Q1, R2 = R3 = Pr]. Hydrogenation of the nitro group (97%) and sulfonamidation of the resultant amino group with 4-cyanobenzenesulfonyl chloride (53%) gave title furandione III, a preferred compd. Several compds. including III are said to have inhibited replication of HIV-1IIIB in human cell lines. HIV-1 protease inhibitory data are provided, and over 100% inhibition was reported for

many test compds. at doses as low as 3.3 .mu.M.

ST tetronic acid prepn antiviral **retrovirus** replication inhibitor;  
furandione prepn antiviral **retrovirus** replication inhibitor;  
HIV protease inhibitor AIDS treatment tetronic acid prepn

IT Human immunodeficiency virus  
Human immunodeficiency virus 1  
(inhibition; prepn. of antiretroviral tetronic acid derivs. for  
treatment of AIDS or AIDS-related diseases)

IT Anti-AIDS agents  
Antiviral agents  
(prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS  
or AIDS-related diseases)

IT AIDS (disease)  
(treatment; prepn. of antiretroviral tetronic acid derivs. for  
treatment of AIDS or AIDS-related diseases)

IT 144114-21-6, Retropepsin  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(inhibitors; prepn. of antiretroviral tetronic acid derivs. for  
treatment of AIDS or AIDS-related diseases)

IT 1138-44-9P 10424-93-8P 72036-34-1P 85520-35-0P 161720-04-3P  
164346-90-1P 164346-91-2P 164346-92-3P 164346-93-4P 164346-94-5P  
164346-95-6P 164346-96-7P 164346-98-9P 164346-99-0P 164347-01-7P  
164347-02-8P 164347-03-9P 164347-07-3P 164347-10-8P 248608-58-4P  
248608-59-5P 248608-60-8P 248608-61-9P 248608-62-0P 248608-63-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(intermediate; prepn. of antiretroviral tetronic acid derivs. for  
treatment of AIDS or AIDS-related diseases)

IT 99-61-6, 3-Nitrobenzaldehyde 100-39-0, Benzyl bromide 103-63-9,  
(2-Bromoethyl)benzene 104-53-0, Hydrocinnamaldehyde 106-94-5  
108-94-1, Cyclohexanone, reactions 109-72-8, n-Butyl lithium, reactions  
120-92-3, Cyclopentanone 502-49-8, Cyclooctanone 623-47-2, Ethyl  
propiolate 637-59-2, 1-Bromo-3-phenylpropane 946-33-8,  
2-Benzylcyclohexanone 1007-03-0, .alpha.-Cyclopropylbenzyl alcohol  
1067-74-9, Methyl diethylphosphonoacetate 2550-26-7, Benzyl acetone  
2637-37-8, 2-Quinolinethiol 4423-94-3, 2-Ethylcyclohexanone 4971-56-6,  
Tetronic acid 14371-10-9 23719-80-4, Cyclopropylmagnesium bromide  
29976-53-2, 1-Carbethoxy-4-piperidone 49584-26-1, 4-Cyanobenzenesulfonyl  
chloride 118753-70-1 135005-10-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant; prepn. of antiretroviral tetronic acid derivs. for treatment  
of AIDS or AIDS-related diseases)

IT 164344-46-1P 164344-47-2P 164344-48-3P 164344-49-4P 164344-50-7P  
164344-51-8P 164344-52-9P 164344-53-0P 164344-54-1P 164344-55-2P  
164344-56-3P 164344-57-4P 164344-58-5P 164344-59-6P 164344-60-9P  
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164344-76-7P 164344-77-8P 164344-79-0P 164344-80-3P 164344-81-4P  
164344-82-5P 164344-83-6P 164344-84-7P 164344-85-8P 164344-86-9P  
164344-87-0P 164344-88-1P 164344-89-2P 164344-90-5P 164344-91-6P  
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164346-35-4P	164346-36-5P	164346-37-6P	164346-38-7P	164346-39-8P
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164346-48-9P	164346-49-0P	164346-50-3P	164346-51-4P	164346-52-5P
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164346-60-5P	164346-61-6P	164346-62-7P	164346-63-8P	164346-64-9P
164346-65-0P	164346-66-1P	164346-67-2P	164346-68-3P	
<b>164346-69-4P</b>	<b>164346-70-7P</b>	<b>164346-71-8P</b>		
164346-72-9P	164346-73-0P	164346-74-1P	164346-75-2P	164346-76-3P
164346-77-4P	164346-78-5P	164346-79-6P	164346-80-9P	
<b>164346-81-0P</b>	<b>164346-82-1P</b>	<b>164346-83-2P</b>		
164346-84-3P	164346-85-4P	164346-86-5P	164346-87-6P	164346-88-7P
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248608-35-7P	248608-36-8P	248608-37-9P	248608-38-0P	248608-39-1P
248608-40-4P	248608-41-5P	248608-42-6P	248608-43-7P	248608-44-8P
248608-45-9P				

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 248608-46-0P 248608-48-2P 248608-49-3P 248608-50-6P 248608-51-7P  
248608-52-8P 248608-53-9P 248608-54-0P 248608-56-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

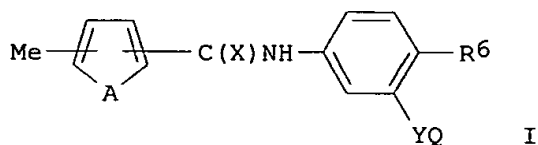
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- (2) Anon
- (3) Anon; 1963
- (4) Anon; 1965
- (5) Anon; 1977 CAPLUS
- (6) Anon; 1979 CAPLUS
- (7) Anon; 1979 CAPLUS
- (8) Anon; 1979 CAPLUS
- (9) Anon; 1982 CAPLUS
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- (14) Anon; JP 04-211676 1992 CAPLUS
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 (33) Roggo, B; J of Antibiotics 1994, V47(2), P143 CAPLUS  
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L12 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2000:784381 CAPLUS  
 DN 133:335153  
 ED Entered STN: 09 Nov 2000  
 TI Preparation of N-arylmethylthioanilide compounds useful for the inhibition  
 of the replication of HIV  
 IN Brouwer, Walter Gerhard; Osika, Ewa Maria  
 PA Uniroyal Chemical Co., Inc., USA; Uniroyal Chemical Co./cie.  
 SO U.S., 9 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A61K031-505  
 ICS A61K031-381; C07D307-68; C07D333-38; C07D405-12  
 NCL 514471000  
 CC 27-6 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 1, 10  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6143780	A	20001107	US 1999-398649	19990917
	WO 2001019811	A2	20010322	WO 2000-US24986	20000912
	WO 2001019811	A3	20010726		
	W: CA				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 1220848	A2	20020710	EP 2000-963380	20000912
	EP 1220848	B1	20031119		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
	AT 254611	E	20031215	AT 2000-963380	20000912
PRAI	US 1999-398649	A	19990917		
	WO 2000-US24986	W	20000912		
OS	MARPAT 133:335153				
GI					



AB The title compds. I [A, X are independently O or S; R6 = H, halo, alkyl, alkoxy, alkylthio, cyano, nitro; Y = CH2O, OCH2, CH2S, CH2SO2; Q = substituted or unsubstituted Ph or arom. heterocyclic group], useful for the inhibition of the replication of **HIV-1** in vitro and in vivo, were prepd. E.g. N-3-((2-chlorophenoxy)methyl)-4-chlorophenyl-2-methyl-3-furancarbothioamide was prepd.

ST arylmethylthioanilide prepn inhibition HIV1; furancarbothioamide prepn inhibition HIV1; furancarboxamide prepn inhibition HIV1

IT Human immunodeficiency virus 1

(prepn. of N-arylmethylthioanilide compds. useful for the inhibition of the replication of **HIV-1**)

IT	255381-42-1P	303964-42-3P	303964-43-4P	303964-44-5P	303964-45-6P
	303964-46-7P	303964-47-8P	303964-48-9P	303964-49-0P	303964-50-3P
	303964-51-4P	303964-52-5P	303964-53-6P	303964-54-7P	303964-55-8P
	303964-56-9P	303964-57-0P	303964-58-1P	303964-59-2P	303964-60-5P
	303964-61-6P	303964-62-7P	303964-63-8P	303964-64-9P	303964-65-0P
	303964-66-1P	303964-67-2P	303964-68-3P	303964-69-4P	303964-70-7P
	303964-71-8P	303964-72-9P	303964-73-0P	303964-74-1P	303964-75-2P
	303964-76-3P	303964-77-4P	303964-78-5P	303964-79-6P	303964-80-9P
	303964-81-0P	303964-82-1P	303964-83-2P	303964-84-3P	303964-85-4P
	303964-86-5P	303964-87-6P	303964-88-7P	303964-89-8P	303964-90-1P
	303964-91-2P	303964-92-3P	303964-93-4P	303964-94-5P	303964-96-7P
	303964-97-8P	303964-98-9P	303964-99-0P	303965-00-6P	303965-01-7P
	303965-02-8P	303965-03-9P	303965-04-0P	303965-05-1P	303965-06-2P
	303965-07-3P	303965-08-4P	303965-09-5P	303965-10-8P	303965-11-9P
	303965-12-0P	303965-13-1P	303965-14-2P	303965-15-3P	
	303965-16-4P	303965-17-5P	303965-28-8P		

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-arylmethylthioanilide compds. useful for the inhibition of the replication of **HIV-1**)

IT 5555-00-0 6361-21-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of N-arylmethylthioanilide compds. useful for the inhibition of the replication of **HIV-1**)

IT 95-57-8P, 2-Chlorophenol 80866-80-4P 124877-63-0P 303965-18-6P  
303965-19-7P 303965-20-0P 303965-21-1P 303965-22-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of N-arylmethylthioanilide compds. useful for the inhibition of the replication of **HIV-1**)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Brouwer; US 5696151 1997 CAPLUS

(2) Brouwer; US 6017947 2000 CAPLUS

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L12 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:695955 CAPLUS

DN 137:232650

ED Entered STN: 13 Sep 2002

TI Preparation of nitrogen-containing heteroaryl compounds having HIV  
 integrase inhibitory activity  
 IN Fuji, Masahiro; Mikamiyama, Hidenori; Murai, Hitoshi  
 PA Shionogi & Co., Ltd., Japan  
 SO PCT Int. Appl., 316 pp.  
 CODEN: PIXXD2

DT Patent

LA Japanese

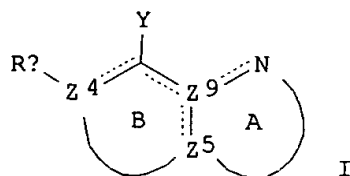
IC ICM C07D215-28

ICS C07D215-48; C07D215-50; C07D235-10; C07D235-08; C07D417-04;  
 C07D417-06; C07D413-04; C07D413-14; C07D491-04; C07D491-048;  
 C07D487-04; C07D513-04; C07D495-04; A61K031-4184; A61K031-427;  
 A61K031-4245; A61K031-422; A61K031-433; A61K031-428

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002070486	A1	20020912	WO 2002-JP1778	20020227
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1375486	A1	20040102	EP 2002-701583	20020227
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	JP 2001-57037	A	20010301		
	JP 2001-243530	A	20010810		
	JP 2001-395022	A	20011226		
	WO 2002-JP1778	W	20020227		
OS	MARPAT 137:232650				
GI					



AB The title compds. I [rings A and B are fused N-contg. heterocyclic rings;  
 Z4, Z5 and Z9 independently represent each carbon or nitrogen; Y  
 represents hydroxy, mercapto or amino; and RA represents nitrogen-contg.  
 heteroaryl, etc.] are prepd. Compds. of this invention in vitro showed  
 IC50 values of 0.11 .mu.g/mL to 0.76 .mu.g/mL against HIV  
 integrase. Formulations are given.  
 ST heteroaryl compd prepn HIV integrase inhibitor  
 IT Enzymes, biological studies  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (prepn. and effect of nitrogen-contg. heteroaryl compds. having  
 HIV integrase inhibitory activity and enzyme inhibitory  
 activity)



IT Salts, preparation  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. and effect of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and salts thereof)

IT Human  
 Solvates  
 (prepn. and effect of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and solvates thereof)

IT AIDS (disease)  
 Anti-AIDS agents  
 (prepn. of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity)

IT Drug delivery systems  
 (prodrugs; prepn. and effect of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and prodrugs thereof)

IT Nucleic acids  
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (related enzymes; prepn. and effect of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and enzyme inhibitory activity)

IT 144114-21-6, **HIV** protease  
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (combination of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and protease inhibitors)

IT 9068-38-6, Reverse transcriptase  
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (combination of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and reverse transcriptase inhibitors)

IT 52350-85-3, **HIV** integrase  
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (of **HIV**; prepn. of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity)

IT 205040-56-8P 410544-61-5P 457945-02-7P 457945-04-9P 457945-05-0P  
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 457945-51-6P 457945-52-7P 457945-53-8P 457945-54-9P 457945-55-0P  
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of nitrogen-contg. heteroaryl compds. having HIV integrase inhibitory activity).

IT 457947-44-3P 457947-45-4P 457947-46-5P 457947-47-6P 457947-48-7P  
457947-49-8P 457947-50-1P 457947-51-2P 457947-52-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of nitrogen-contg. heteroaryl compds. having HIV integrase inhibitory activity)

IT 64-17-5, Ethanol, reactions 74-88-4, Methyl iodide, reactions 74-89-5, Methylamine, reactions 74-96-4, Ethyl bromide 75-07-0, Acetaldehyde, reactions 75-16-1, Methylmagnesium bromide 75-31-0, Isopropylamine, reactions 75-36-5, Acetyl chloride 77-78-1, Dimethyl sulfate 85-38-1 87-13-8, Diethyl ethoxymethylenemalonate 90-04-0, 2-Methoxyaniline 96-33-3, Methyl acrylate 98-80-6, Phenylboronic acid 100-39-0, Benzyl bromide 100-46-9, Benzylamine, reactions 103-72-0, Phenylthioisocyanate 107-21-1, Ethylene glycol, reactions 107-30-2, Methoxymethyl chloride 108-24-7, Acetic anhydride 123-62-6, Propionic anhydride 124-38-9, Carbon dioxide, reactions 124-40-3, Dimethylamine, reactions 124-41-4, Sodium methoxide 288-32-4, Imidazole, reactions 302-01-2, Hydrazine, reactions 334-88-3, Diazomethane 405-50-5, p-Fluorophenylacetic acid 431-03-8, Diacetyl 459-04-1, 4-Fluorophenylacetyl chloride 459-32-5 459-46-1, 4-Fluorobenzyl bromide 462-08-8, 3-Aminopyridine 501-52-0, Benzenepropanoic acid 506-59-2, Dimethylamine hydrochloride 506-68-3, Bromocyanide 521-74-4 544-92-3, Copper cyanide 607-35-2 630-08-0, Carbon monoxide, reactions 824-79-3, Sodium p-toluenesulfinate 937-39-3, Phenylacetylhydrazide 1066-54-2, Trimethylsilylacetylene 1117-97-1, N,O-Dimethylhydroxylamine 1461-22-9, Tributyltin chloride 2127-03-9, 2,2'-Dipyridyldisulfide 2533-69-9, Methyl 2,2,2-trichloroacetimidate 2591-86-8, N-Formylpiperidine 3034-53-5, 2-Bromothiazole 4595-60-2, 2-Bromopyrimidine 4637-24-5, Dimethylformamide dimethylacetal 5419-55-6, Triisopropyl borate 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 7486-35-3, Tributylvinylstannane 7553-56-2, Iodine, reactions 7640-33-7 7664-41-7, Ammonia, reactions 7726-95-6, Bromine, reactions 12125-02-9, Ammonium chloride, reactions 19829-79-9 31230-17-8 34547-28-9 51110-60-2 56826-69-8 64214-66-0 73183-34-3, Bis(pinacolato)diborane 76513-69-4, 2-(Trimethylsilyl)ethoxymethyl chloride 91478-74-9 93102-98-8,

1-Amino-3-(4-fluorophenyl)propan-2-one hydrochloride 107095-99-8  
115192-48-8 126463-85-2 126463-87-4 145837-83-8 154355-81-4,  
2-Bromo-5-(p-fluorobenzyl) furan 199931-43-6 280572-13-6 457947-54-5  
457947-55-6 457947-56-7 457947-57-8 457947-58-9 457947-60-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of nitrogen-contg. heteroaryl compds. having HIV  
integrase inhibitory activity)

IT 459-31-4P, 4-Fluorobenzenepropanoic acid 5129-25-9P 5341-07-1P  
7175-09-9P 14151-06-5P 17012-49-6P 20075-26-7P 63416-70-6P  
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(prepn. of nitrogen-contg. heteroaryl compds. having HIV  
integrase inhibitory activity)

IT 459476-94-9 459476-95-0 459476-96-1 459476-97-2

RL: PRP (Properties)

(unclaimed sequence; prepn. of nitrogen-contg. heteroaryl compds.  
having HIV integrase inhibitory activity)

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RE

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=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	14.93	361.65
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.77	-4.85

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 DICTIONARY FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> S 457949-18-7/RN

L14 1 457949-18-7/RN

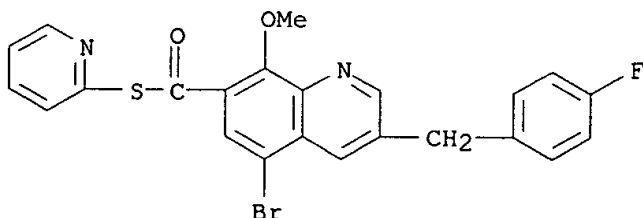
=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> D L14 SQIDE 1-

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THE ESTIMATED COST FOR THIS REQUEST IS 5.92 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 457949-18-7 REGISTRY  
CN 7-Quinolinecarbothioic acid, 5-bromo-3-[(4-fluorophenyl)methyl]-8-methoxy-, S-2-pyridinyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H16 Br F N2 O2 S  
SR CA  
LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

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=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.19	363.84
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

CA SUBSCRIBER PRICE

ENTRY      SESSION  
0.00      -4.85

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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4  
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l11 and l10  
L15            5 L11 AND L10

=> s l15 not l12  
L16            2 L15 NOT L12

=> d l16 1-2

L16 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1999:561590 CAPLUS  
DN 131:184948  
TI Preparation of benzimidazolylsulfinylmethylarylamines as (H<sup>+</sup>/K<sup>+</sup>) ATPase inhibitors useful as antiviral agents.  
IN Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil, Clara I.  
PA G.D. Searle & Co., USA  
SO U.S., 54 pp., Cont.-in-part of Ser. No. US 1994-  
CODEN: USXXAM  
DT Patent  
LA English  
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	US 5945425	A	19990831	US 1996-737251	19961024
	WO 9529897	A1	19951109	WO 1995-US5021	19950501
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 2001047038	A1	20011129	US 2001-885221	20010620
PRAI	US 1994-235619	B2	19940429		
	WO 1995-US5021	W	19950501		
	US 1996-659098	B1	19960604		

US 1999-377888 B1 19990819  
US 2000-605560 B1 20000627

OS MARPAT 131:184948

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1970:111444 CAPLUS

DN 72:111444

TI Antiviral and neuroleptic .alpha.-carbolines

PA Glaxo Laboratories Ltd.

SO Fr. Demande, 52 pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2003999		19691114		
	DE 1913119			DE	
	GB 1268772			GB	
	ZA 6901818		19690000	ZA	
PRAI	GB		19680315		

=> d 116 1 all

L16 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:561590 CAPLUS

DN 131:184948

ED Entered STN: 03 Sep 1999

TI Preparation of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase inhibitors useful as antiviral agents.

IN Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil, Clara I.

PA G.D. Searle & Co., USA

SO U.S., 54 pp., Cont.-in-part of Ser. No. US 1994-

CODEN: USXXAM

DT Patent

LA English

IC ICM A61K031-42

ICS A61K031-415; A61K031-425

NCL 514269000

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5945425	A	19990831	US 1996-737251	19961024
	WO 9529897	A1	19951109	WO 1995-US5021	19950501
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 2001047038	A1	20011129	US 2001-885221	20010620
PRAI	US 1994-235619	B2	19940429		
	WO 1995-US5021	W	19950501		
	US 1996-659098	B1	19960604		
	US 1999-377888	B1	19990819		

US 2000-605560 B1 20000627

OS MARPAT 131:184948

AB A method of treating viral infection comprises treatment with R2(CR3R4)pSOM(CR4R5)nR1 [R1 = (substituted) alkoxy, alkoxy carbonyl, dialkylamino, aryl, heteroaryl; R2 = (substituted) heteroaryl; R3-R6 = H, alkyl, aryl, aralkyl; R3R4, R5R6 = cycloalkyl; m, n, p = 0-2]. Thus, 2-mercaptobenzimidazole and 2-aminobenzyl alc. were heated in HOAc/H<sub>2</sub>SO<sub>4</sub> to give 2-[(1H-benzimidazol-2-yl)thiomethyl]benzeneamine. The latter in CHCl<sub>3</sub> was treated with 2-[(1H-benzimidazol-2-yl)sulfinylmethyl]benzeneamine. Title compds. inhibited **HCMV** replication with EC<sub>50</sub> = 13-61 .mu.M.

ST benzimidazolylsulfinylmethylarylamines prepn ATPase inhibitor antiviral  
IT Antiviral agents

(prepn. of benzimidazolylsulfinylmethylarylamines as (H<sup>+</sup>/K<sup>+</sup>) ATPase inhibitors useful as antiviral agents)

IT	100924-68-3P	104340-33-2P	104340-34-3P	104340-35-4P	104340-37-6P
	104340-38-7P	104524-67-6P	104524-68-7P	106746-58-1P	106746-60-5P
	106746-61-6P	106746-63-8P	106746-65-0P	106746-66-1P	106746-68-3P
	106746-69-4P	106746-76-3P	106746-77-4P	106746-78-5P	106746-79-6P
	106746-80-9P	106746-84-3P	106746-86-5P	106746-88-7P	106746-90-1P
	106746-93-4P	106746-94-5P	106746-95-6P	106746-96-7P	106746-97-8P
	106746-98-9P	106747-00-6P	106747-05-1P	106747-06-2P	106747-07-3P
	106747-08-4P	106747-10-8P	106747-11-9P	106747-12-0P	106747-13-1P
	106747-14-2P	106747-15-3P	106747-16-4P	106747-17-5P	106747-18-6P
	106747-19-7P	106747-20-0P	106747-21-1P	106747-22-2P	106747-23-3P
	106747-24-4P	106747-25-5P	106747-26-6P	106747-27-7P	106747-28-8P
	106747-29-9P	106747-30-2P	106747-31-3P	106747-32-4P	106747-33-5P
	106747-34-6P	106747-35-7P	106747-36-8P	106747-38-0P	106747-39-1P
	106747-40-4P	106747-41-5P	106747-42-6P	106747-43-7P	106747-44-8P
	106747-45-9P	106747-47-1P	106747-48-2P	106771-58-8P	106785-95-9P
	106785-96-0P	108542-64-9P	108542-66-1P	111477-14-6P	111502-75-1P
	114060-19-4P	118267-21-3P	118267-22-4P	118267-23-5P	118267-24-6P
	118267-25-7P	118267-26-8P	118267-27-9P	118267-28-0P	118267-29-1P
	118267-30-4P	118267-33-7P	118267-34-8P	118267-35-9P	118267-36-0P
	118267-37-1P	118267-38-2P	118267-39-3P	118267-42-8P	118267-43-9P
	118292-92-5P	118292-93-6P	118292-94-7P	118292-95-8P	118292-96-9P
	118292-97-0P	118292-98-1P	118292-99-2P	174397-92-3P	174397-93-4P
	174397-94-5P	174397-95-6P	174397-96-7P	174397-97-8P	174397-98-9P
	174397-99-0P	174398-00-6P	174398-01-7P	174398-02-8P	174398-03-9P
	174398-04-0P	174398-05-1P			

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolylsulfinylmethylarylamines as (H<sup>+</sup>/K<sup>+</sup>) ATPase inhibitors useful as antiviral agents)

IT	55546-06-0	56713-45-2	57235-18-4	60524-97-2	71670-48-9
	73590-36-0	73590-58-6	73590-61-1	81527-04-0	81864-40-6
	81864-65-5	94452-40-1	96733-60-7	96831-93-5	97288-52-3
	97963-93-4	97966-85-3	98412-35-2	98412-41-0	99153-80-7
	99499-40-8	101387-97-7	102127-07-1	102127-11-7	102625-54-7
	102625-70-7	102625-79-6	103014-24-0	103577-45-3	103922-27-6
	103971-24-0	104340-41-2	104340-85-4	104658-07-3	104685-57-6
	104987-90-8	105389-59-1	105950-65-0	105982-35-2	106747-09-5
	107512-17-4	108026-58-0	108499-76-9	108662-50-6	109827-59-0
	110405-59-9	110754-85-3	111371-25-6	111371-35-8	111476-81-4
	111476-82-5	111476-83-6	111476-84-7	111476-85-8	111476-86-9
	111476-87-0	111476-88-1	111476-89-2	111476-91-6	111476-92-7
	111476-93-8	111476-94-9	111476-95-0	111476-96-1	111476-97-2
	111476-98-3	111476-99-4	111477-01-1	111477-02-2	111477-03-3
	111477-04-4	111604-52-5	111604-57-0	111858-83-4	112058-72-7
	112058-73-8	112230-13-4	112645-53-1	112705-43-8	113209-69-1
	113418-90-9	113703-12-1	113703-14-3	113703-20-1	113703-21-2



113703-22-3	113703-28-9	113712-97-3	113805-04-2	113855-38-2
113855-39-3	113855-40-6	113855-41-7	113855-42-8	113915-02-9
113942-61-3	114560-55-3	114878-71-6	115046-03-2	115366-78-4
115366-80-8	116091-77-1	116940-41-1	117038-05-8	117046-87-4
117347-86-1	117426-13-8	117934-10-8	117977-41-0	120009-37-2
120393-57-9	120699-85-6	120699-91-4	120894-71-5	121050-40-6
121242-23-7	121591-86-4	122307-32-8	122508-81-0	123215-59-8
123215-83-8	123451-58-1	123823-95-0	123907-70-0	123987-02-0
124736-45-4	124899-76-9	125214-42-8	126026-46-8	128429-74-3
128935-96-6	128936-05-0	130049-59-1	130368-60-4	130368-62-6
130368-66-0	133903-90-9	134017-66-6	134462-81-0	135430-38-5
135461-65-3	135863-25-1	137105-02-3	137247-56-4	137810-46-9
139644-93-2	139767-99-0	142062-72-4	150064-18-9	150460-06-3
153284-85-6	174398-06-2	174398-07-3	174398-08-4	174398-09-5
174398-10-8	174398-12-0	174398-13-1	174398-15-3	174398-20-0
187589-30-6	240118-16-5	240118-17-6		

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(prepn. of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase inhibitors useful as antiviral agents)

IT 366-18-7, 2,2'-Dipyridyl 400-98-6, 4-Trifluoromethyl-2-nitroaniline  
 446-33-3, 3-Fluoro-6-nitrotoluene 452-71-1, 4-Fluoro-2-methylaniline  
 455-14-1, 4-Trifluoromethylaniline 496-72-0, 3,4-Diaminotoluene  
 570-24-1, 2-Methyl-6-nitroaniline 583-39-1, 2-Mercaptobenzimidazole  
 616-86-4, 4-Ethoxy-2-nitroaniline 1603-41-4, 2-Amino-5-methylpyridine  
 1635-61-6, 3-Chloro-6-nitroaniline 1635-84-3, 2,4-Dimethyl-6-nitroaniline  
 1639-31-2, 3,4,5-Trimethylaniline 1824-81-3, 2-Amino-6-methylpyridine  
 3171-45-7, 4,5-Dimethyl-1,2-phenylenediamine 5327-33-3, 2-Acetamido-6-methylpyridine  
 5344-90-1, 2-Aminobenzyl alcohol 7595-31-5, 3,4-Dimethoxy-6-nitroaniline  
 23019-47-8 23612-57-9 27492-84-8, Methyl 4-amino-2-methoxybenzoate 37052-78-1, 2-Mercapto-5-methoxybenzimidazole  
 39785-37-0, 4-Methoxy-3,5-dimethylaniline 59338-85-1 61713-46-0 71675-52-0 71693-08-8 88301-76-2  
 88301-77-3 88301-78-4 88301-79-5 88301-81-9, 2-Chloromethylaniline hydrochloride  
 92333-53-4 92807-01-7 106746-59-2, 2-Chloromethyl-4-methoxyaniline hydrochloride  
 106746-62-7 106746-64-9 106746-67-2 106746-71-8 106746-73-0 106746-83-2  
 106746-85-4 106746-87-6 106746-89-8 106746-91-2 106746-92-3 106746-99-0  
 106771-59-9, 2-Chloromethyl-N,N-dimethylaniline 118267-31-5 174397-87-6  
 174397-89-8 175276-96-7 240118-15-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase inhibitors useful as antiviral agents)

IT 3287-79-4P, 5,6-Dimethyl-2-mercaptobenzimidazole 4093-29-2P, Methyl 4-acetamido-2-methoxybenzoate  
 25369-78-2P 25617-34-9P 27231-33-0P 55489-15-1P 59338-84-0P 73590-92-8P 74004-74-3P, 2-Mercapto-5,6-dimethoxybenzimidazole  
 86604-73-1P 86847-79-2P 106746-72-9P 106746-74-1P 106746-75-2P 106746-81-0P 106746-82-1P  
 106747-02-8P 106747-03-9P 106747-04-0P 106747-46-0P 106771-57-7P 118267-40-6P 118267-41-7P  
 174397-86-5P 174397-90-1P 174397-91-2P 174398-21-1P 174398-22-2P 240118-07-4P 240118-08-5P 240118-09-6P  
 240118-11-0P 240118-12-1P 240118-13-2P 240118-14-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase inhibitors useful as antiviral agents)

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD

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=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	5.85	369.69
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.69	-5.54

FILE 'REGISTRY' ENTERED AT 09:49:33 ON 21 JAN 2004  
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STRUCTURE FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4  
DICTIONARY FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> S 174398-05-1/RN

L17 1 174398-05-1/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=>

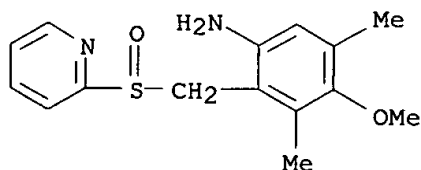
=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> D L17 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y  
THE ESTIMATED COST FOR THIS REQUEST IS 5.92 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L17 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 174398-05-1 REGISTRY  
CN Benzenamine, 4-methoxy-3,5-dimethyl-2-[(2-pyridinylsulfinyl)methyl]- (9CI)  
(CA INDEX NAME)  
FS 3D CONCORD  
MF C15 H18 N2 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=>

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.19	371.88
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-5.54

FILE 'CAPLUS' ENTERED AT 09:50:25 ON 21 JAN 2004  
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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4  
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004

L1 STRUCTURE UPLOADED  
L2 0 S L1 EXA SAM  
L3 0 S L1 FAM SAM  
L4 50 S L1 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004

L5 10 S L4

FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004

L6 4073 S L1 SSS FULL  
L7 3719 S HIV OR RETROVIRAL OR RETROVIRUS  
L8 2422 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004  
L9 70667 S HIV OR RETROVIRAL OR RETROVIRUS  
L10 31317 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV  
L11 636 S L6  
L12 9 S L11 AND L9

FILE 'REGISTRY' ENTERED AT 09:41:14 ON 21 JAN 2004  
L13 1 S 188839-16-9/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:42:34 ON 21 JAN 2004

FILE 'REGISTRY' ENTERED AT 09:47:14 ON 21 JAN 2004  
L14 1 S 457949-18-7/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:48:05 ON 21 JAN 2004  
L15 5 S L11 AND L10  
L16 2 S L15 NOT L12

FILE 'REGISTRY' ENTERED AT 09:49:33 ON 21 JAN 2004  
L17 1 S 174398-05-1/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:50:25 ON 21 JAN 2004

=> d l16 2 all

L16 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1970:111444 CAPLUS  
DN 72:111444  
ED Entered STN: 12 May 1984  
TI Antiviral and neuroleptic .alpha.-carbolines  
PA Glaxo Laboratories Ltd.  
SO Fr. Demande, 52 pp.  
CODEN: FRXXBL  
DT Patent  
LA French  
IC A61K; C07D  
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	FR 2003999		19691114		
	DE 1913119			DE	
	GB 1268772			GB	
	ZA 6901818		19690000	ZA	
PRAI	GB		19680315		

GI For diagram(s), see printed CA Issue.

AB The 2-substituted .alpha.-carbolines (I) in which X is other than a halogen atom or an acyloxy group are prepd. by reaction of a salt (II) or a compd. (III) with a reactive nucleophile. Thus, 2 g 1-methoxy-.alpha.-carbolinium methyl sulfate (IV) heated in a sealed tube at 110.degree. with 35 ml aq. NH4OH (d. 0.88) 4 hr gave 0.27 g unidentified compd. and further eluted with C6H6 contg. 50% AcOEt gave 38% 2-amino-.alpha.-carboline, m. 202-3.degree.. Similarly was obtained 2-hydrazino-.alpha.-

carboline, m. 185-7.degree.. Analogous treatment of IV provided I (R = H) (X and m.p. given): NHMe, 156-7.degree.; CN, 289-91.degree.; OMe, 167-9.degree.; SPh, 222-3.degree.; OCH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 117-19.degree.; HNCH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 102-3.degree.; SCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Me, 179.0-8095.degree.; SCH<sub>2</sub>Ph, 182.5-3.0.degree.; SCH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 137.9.degree.; HN-(CH<sub>2</sub>)<sub>3</sub>Me, 154-6.degree.; CH<sub>2</sub>CO<sub>2</sub>Et, 208-10.degree.; CH<sub>2</sub>CO<sub>2</sub>Et, 200-2.degree.; morpholino, 263-5.degree.; OH, 295.degree. (decompn.). Treatment of 0.9 g 1-methoxy-9-methyl-.alpha.-carbolinium methyl sulfate (V) in 5 ml H<sub>2</sub>O with 0.5 g KCN in 2 ml H<sub>2</sub>O yielded I (R = Me, X = C N), m. 152-63.degree.. V in H<sub>2</sub>O stirred 2 hr with 40% aq. NaOH and the filtered soln. neutralized with 2N HCl yielded 34% I (R = Me, X = OH), m. 266-8.degree.. Dry PhMe (50 ml) contg. 3 g 1-ethoxy-.alpha.-carbolinium tetrafluoroborate, and 3.75 g. H<sub>2</sub>NCH<sub>2</sub>-CHMeOH refluxed 5 hr gave 0.32 g I (R = H, X = NHC h<sub>2</sub>CH-MeOH), m. 185-7.degree. (AcOEt). Similarly was obtained I (R = H, X = NH(CH<sub>2</sub>)<sub>3</sub>OH), m. 163-6.degree.. AcCH<sub>2</sub>CO<sub>2</sub>Et (4 ml) and 1-methoxy-.alpha.-isocarboline (from 1 g V) heated 2.5 hr on a steam bath and the cooled product treated with H<sub>2</sub>O gave 18.5 % I (R = H, X = CH<sub>2</sub>CO<sub>2</sub>Et), m. 200-2.degree.. Similarly were prepd. I (R = H, X = CH<sub>2</sub>COMe), m. 205-7.degree.; I (R = H, X = CH-(CN)<sub>2</sub>), m. 296-7.degree., and I (R = H, X = OMe), m. 166-9.degree., in 24, 12, and 23% yields. HO(CH<sub>2</sub>)<sub>5</sub>NH<sub>2</sub> (30 ml) and 12 g 2-chloro-9-methyl-.alpha.-carboline heated in a sealed tube 16 hr at 200.degree. and the product partitioned between C<sub>6</sub>H<sub>6</sub> and 2N aq. Na<sub>2</sub>CO<sub>3</sub>, the C<sub>6</sub>H<sub>6</sub> ext. shaken with excess 2N HCl and filtered gave the HCl salt of I [R = Me, X = NH(CH<sub>2</sub>)<sub>5</sub>OH], m. 200-2.degree.. A mixt. of 10 g o-H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> and 25 g 2,6-Br<sub>2</sub>C<sub>5</sub>H<sub>3</sub>N heated 8 hr at 140.degree. and the product partitioned between CHCl<sub>3</sub> and aq. Na<sub>2</sub>CO<sub>3</sub>, the C<sub>6</sub>H<sub>6</sub> ext. shaken with excess 2N HCl and filtered gave the HCl salt of I [R = Me, X = NH(CH<sub>2</sub>)<sub>5</sub>OH], m. 200-2.degree.. A mixt. of 10 g o-H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> and 25 g 2,6-Br<sub>2</sub>C<sub>5</sub>H<sub>3</sub>N heated 8 hr at 140.degree. and the product partitioned between CHCl<sub>3</sub> and aq. Na<sub>2</sub>CO<sub>3</sub>, the CHCl<sub>3</sub> layer evapd. and the residue taken up on 500 g silica gel, eluted with C<sub>6</sub>H<sub>6</sub> contg. increasing amts. of EtOAc gave 21 g unchanged 2,6-Br<sub>2</sub>C<sub>5</sub>H<sub>3</sub>N and 2.2 g 2-(o-amino anilino)-6-bromopyridine (VI), m. 141-2.degree. (iso-PrOH). VI (2.2 g) in 20 ml EtOH and 30 ml 5N HCl treated at 0.degree. with 1.03 g NaNO<sub>2</sub> in 12 ml H<sub>2</sub>O gave 2.27 g 1-(6-bromopyrid-2-yl)benzo-triazole (VII), m. 115-16.degree. (EtOH). Benzotriazole (1 g) and 2 g 2,6-Br<sub>2</sub>C<sub>5</sub>H<sub>3</sub>N heated 5 min at 210.degree. with evolution of HBr and the cooled gum extd. with petroleum ether yielded 0.55 g VII. VII (3.5 g) and 20 g polyphosphoric acid heated 6 hr at 130.degree. and the cooled mixt. poured into H<sub>2</sub>O, filtered and the dried ppt. crystd. from C<sub>6</sub>H<sub>6</sub> gave 0.95 g I (R = H, X = Br) (VIII), m. 290.degree.. Benzotriazole (17.8 g) and 22.2 g 2,6-Cl<sub>2</sub>C<sub>5</sub>H<sub>3</sub>N heated 2 hr at 215.degree. (N atm.) and the cooled product extd. with 800 ml hot C<sub>6</sub>H<sub>12</sub> gave 16 g 1-(6-chloropyrid-2-yl)benzotriazole (IX), m. 130-1.degree.. Polyphosphoric acid (400 g) stirred at 180.degree. with addn. of 75 g IX and the mixt. kept 30 min at 160.degree., poured into 1 l. H<sub>2</sub>O and the dried ppt. crystd. in BuOAc gave 13.8 g I (R = H, X = Cl) (X) m. 271-3.degree.. X (5.06 g) in 120 ml MeO-CH<sub>2</sub>CH<sub>2</sub>OMe stirred with 0.72 g NaH 2.25 hr and the pale yellow soln. kept 2.5 hr at 20.degree. with 4.26 g MeI gave 3.8 g I (R = Me, X = Cl) (XI), m. 126-8.degree.. The 2-halo-substituted compds. VIII, X, and XI heated with the nucl eophilic reagent under the specified conditions of time and temp. in a sealed tube (if necessary) gave the following I (R = H) (X and m.p. given): O(CH<sub>2</sub>)<sub>3</sub>Me, 178-9.degree.; O(CH<sub>2</sub>)<sub>2</sub>OH, 172-4.degree.; O(CH<sub>2</sub>)<sub>3</sub>OH, 178-9.degree.; O(CH<sub>2</sub>)<sub>2</sub>O(CH<sub>2</sub>)<sub>2</sub>OH, 147-9.degree.; [O(CH<sub>2</sub>)<sub>2</sub>]<sub>3</sub>OH, 100-1.degree.; NH<sub>2</sub>, 198-9.degree.; NH(CH<sub>2</sub>)<sub>3</sub>Me, 154-6.degree.; NH(CH<sub>2</sub>)<sub>7</sub>Me, 135-6.degree.; NEt<sub>2</sub>, -; morpholino, 263-5.degree.; 4-methylpyridazin-1-yl, 295-9.degree.; NHPh, 216-17.degree.; NH(CH<sub>2</sub>)<sub>2</sub>-OH, 180-3.degree.; NH(CH<sub>2</sub>)<sub>3</sub>OH, 167-9.degree.; NH(CH<sub>2</sub>)<sub>5</sub>OH, 137-8.degree.; NH(CH<sub>2</sub>)<sub>6</sub>OH, 155-7.degree.; NHCH<sub>2</sub>CH(OH)Me, 186-7.degree.; NH-(CH<sub>2</sub>)<sub>3</sub>OMe, 103-4.degree.; and also I (R = Me) (X and m.p. given): NHMe, 243-6.degree.; NH(CH<sub>2</sub>)<sub>3</sub>Me, 166-8.degree.; NH(CH<sub>2</sub>)<sub>5</sub>OH, 192-4.degree.; HNCH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 211-15.degree.. POCl<sub>3</sub> (5.2 ml) stirred 30 min with 6.2 g 4-chloro-.alpha.-carboline 1-oxide in 60 ml HCONMe<sub>2</sub> and the

mixt. heated 45 min on a steam bath, kept 18 hr at 20.degree. and poured into 500 ml H<sub>2</sub>O, neutralized with Na<sub>2</sub>CO<sub>3</sub> and the ppt. crystd. from 100 ml MeOCH<sub>2</sub>CH<sub>2</sub>OH; the cryst. product (4.78 g) digested 1 hr in 60 ml EtOH and 60 ml 2N NaOH on a steam bath and dild. with H<sub>2</sub>O gave 4.38 g 2,4-dichloro-.alpha.-carboline (XII), m. 305-7.degree. (MeOCH<sub>2</sub>CH<sub>2</sub>OH). XII (0.5 g) and 7 ml BuNH<sub>2</sub> heated in a sealed tube 19 hr at 200.degree. and the cooled mixt. freed from solvent, the dried residue triturated with dil. aq. Na<sub>2</sub>CO<sub>3</sub> and the product recrystd. gave 0.48 g 2,4-di(butyl-amino)-.alpha.-carboline, m. 163-5.degree.. X (2.02 g) and 0.66 g NaH stirred 15 min in 40 ml MeCH(OMe)<sub>2</sub> and the mixt. refluxed 8 hr with 5.3 g Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>Cl in 30 ml C<sub>6</sub>H<sub>6</sub>, the residue on evapn. partitioned between C<sub>6</sub>H<sub>6</sub> and H<sub>2</sub>O and the C<sub>6</sub>H<sub>6</sub> layer evapd., the yellow gum (2.5 g) taken up in 10 ml EtOH and acidified with alc. HBr gave 2.2 g I[R = Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>, X = Cl], HBr salt m. 215-18.degree. (alc.). Conversion of X by the above procedures gave I(R = H, X = SCH<sub>2</sub>CH<sub>2</sub>Me), m. 197-8.degree. (iso-PrOH) and I(R = Pr, X = Cl) (XIII), m. 77-8.degree. (iso-PrOH). XIII (1.09 g) and 6 ml BuO(CH<sub>2</sub>)<sub>3</sub>NH<sub>2</sub> heated 16 hr at 200.degree. in a sealed tube gave I[R = Pr, X = NH(CH<sub>2</sub>)<sub>3</sub>OH], m. 89-91.degree. (Et<sub>2</sub>O) and I[R = Pr, X = NH(CH<sub>2</sub>)<sub>3</sub>OCHMe<sub>2</sub>], HBr salt m. 111-12.degree. (EtOAc). XII (0.5 g), 7 ml HCONMe<sub>2</sub>, and 0.5 ml POCl<sub>3</sub> heated 1 hr on a steam bath and mixt. poured into 25 ml H<sub>2</sub>O gave 0.504 g solid. The solid (0.25 g) extd. by 30 ml 2:1 C<sub>6</sub>H<sub>12</sub>-C<sub>6</sub>H<sub>6</sub> gave 2,4-dichloro-9-formyl-.alpha.-carboline, m. 150.0-60.5.degree.. PhNHMe (345 ml), 1.2 kg 2,6,3-Cl<sub>2</sub>(O<sub>2</sub>N)C<sub>5</sub>H<sub>2</sub>N, and 320 g NaHCO<sub>3</sub> refluxed 2 hr in 10 l. EtOH and the hot filtered soln. cooled gave 1.142 kg 6-chloro-2-(N-methylanilino)-3-nitropyridine (XIV), m. 75-7.degree.. XIV (0.73 g) in 10 ml 10% aq. AcOH kept 30 min at 80.degree. with 3 g powd. Fe, the mixt. basified with aq. Na<sub>2</sub>CO<sub>3</sub>, and extd. with C<sub>6</sub>H<sub>6</sub> gave 0.36 g 3-amino-6-chloro-2-(N-methylanilino)pyridine (XV), m. 94-7.degree.. XV (1.17 g) in 94 ml H<sub>2</sub>O and 12 ml H<sub>2</sub>SO<sub>4</sub> treated dropwise at 5.degree. with 0.37 g NaNO<sub>2</sub> in 10 ml H<sub>2</sub>O, the mixt. treated in 15 min with 4 g powd. Cu with heating to 45.degree., and extd. with EtOAc gave XI. Conversion of XI yielded I[R = Me, X = HO(CH<sub>2</sub>)<sub>3</sub>O], m. 74-6.degree.; I[R = Me, X = H<sub>2</sub>N(CH<sub>2</sub>)<sub>6</sub>NH](2HBr salt m. 251-3.degree.); I(R = Me, X = PhNH), m. 132-3.degree. (iso-PrOH). XI (5 g) shaken 18 hr with 10 ml concd. HNO<sub>3</sub> (d. 1.42) and the mixt. poured into H<sub>2</sub>O yielded 58% 2-chloro-6-nitro-.alpha.-carboline (XVI), m. >410.degree.. Conversion of XVI yielded 29% 2-butylamino-6-nitro-.alpha.-carboline m. 189-90.degree. (CHCl<sub>3</sub>); 32% 2-[2-(diethylamino)ethylamino]-6-nitro-.alpha.-carboline, m. 170-5.degree.; and 62% 9-benzyl-2-chloro-6-nitro-.alpha.-carboline, m. 220.degree. (EtOAc), further transformed to 63% 9-benzyl-2-butylamino-6-nitro-.alpha.-carboline, m. 131-2.degree.. XI (3.5 g) in 40 ml CCl<sub>4</sub> and 10 ml CHCl<sub>3</sub> stirred 1 hr with 1.71 g Cl in CCl<sub>4</sub> and treated with 30 ml 2N NaOH yielded 18% 2,6-dichloro-9-methyl-.alpha.-carboline (XVII), m. 188-90.degree. (ligroine). XVII (350 mg) and 2.5 ml BuNH<sub>2</sub> heated 16 hr at 200.degree. in a sealed tube and the product partitioned between EtOAc and H<sub>2</sub>O, the EtOAc layer evapd. and the oil treated with alc. HCl and Et<sub>2</sub>O gave 0.4 g 2-butylamino-6-chloro-1-methyl-.alpha.-carboline-HCl, m. 194-6.degree. (alc.). XI was similarly converted to 6-chloro-2-(5-hydroxypentylamino)-9-methyl-.alpha.-carboline-HCl, m. 213.5-15.5.degree. (alc.). XVI reduced with NaH in dry glyme and treated with MeI gave 2-chloro-9-methyl-6-nitro-.alpha.-carboline, m. 269-71.degree. (BuOAc), converted to 2-butylamino-9-methyl-6-nitro-.alpha.-carboline, m. 90.degree. [(iso-Pr)<sub>2</sub>O]. [R = Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>, X = Cl] HBr salt heated with BuNH<sub>2</sub> at 210.degree. and the product treated with alc. HBr gave I[R = Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>, X = BuNH<sub>2</sub>].2HBr, m. 213-16.degree.. I(R = H, X = MeNH), HCl salt (0.47 g) in 30 ml H<sub>2</sub>O basified with 4 ml 2N NaOH and extd. with EtOAc, the product taken up in 30 ml EtOH and refluxed 19 hr with 0.52 g morpholine and 0.67 ml 36% formol, the oily product taken up in 30 ml alc. and treated with the same amts. of morpholine and formol, refluxed 24 hr and the product extd. with Et<sub>2</sub>O yielded 38% I(R = N-morpholinomethyl, X = MeNH), m. 220.degree.. Hydrogenation of 250 mg 2-anilino-6-chloro-3-nitropyridine, m. 102-4.degree., in 25 ml EtOAc in the presence of 90 mg

10% Pd-C gave 238 mg 3-amino-2-anilino-6-chloropyridine, diazotized to give 50 mg 5-chloro-3-phenyltriazolo[4,5-b]pyridine, heated at 200.degree. with 0.3 g polyphosphoric acid to yield 3 mg X. Ac2O (40 ml) contg. 4 g .alpha.-carboline 1-oxide refluxed 30 min gave I (R = Ac, X = AcO), m. 155-7.degree., refluxed with aq NaOH and acidified with HCl to give 2-hydroxy-.alpha.-carboline, m. 294.degree. (decompn.), acetylated to 2-ace-toxy-.alpha.-carboline, m. 210.degree.. XII (2.4 g) in 100 ml MeOCH2CH2-OMe stirred 2 hr at 20.degree. with 0.338 g NaH and the soln. stirred 2 hr with 0.69 ml MeI, evapd. and the residue dild. with H2O gave 2.48 g 2,4-dichloro-9-methyl-.alpha.-carboline, m. 178-9.degree. (EtOAc). XI heated with BuNH2 at 200.degree. and the HCl salt crystd. from EtOH gave I (R = Me, X = BuNH) HCl salt monoethanolate, dried 8 hr at 60 .degree./0.1 mm to yield the nonsolvated salt, m. 166-8.degree.. NaHCO3 (480 mg), 554 mg p-MeC6H4NH2 and 1 g 2,6-dichloro-3-nitropyridine refluxed 1 hr in 15 ml EtOH yielded 800 mg 6-chloro-3-nitro-2-(p-toluidino)pyridine, m. 116-19.degree. (iso-PrOH), converted by stirring with NaH in glyme and refluxing the soln. with MeI to give 400 mg 6-chloro-2-(N-methyl-p-toluidino)-3-nitropyridine, m. 113-15.degree., reduced with powd. Fe in boiling AcOH to the corresponding 3-amino-6-chloro-2-(N-methyl-p-toluidino)pyridine (XVIII), m. 90-1.degree.. XVIII (750 mg) diazotized in 8 ml concd. H2SO4 and 8 ml H2O at 6.degree. with 230 mg NaNO2 in 4 ml H2O, stirred 1.5 hr with gradual addn. of 600 mg pptd. Cu and extd. with CHCl3 gave 500 mg 2-chloro-6,9-dimethyl-.alpha.-carboline, m. 132-4.degree. [(Me2CH)2O], converted to the corresponding 2-butylamino-6,9-dimethyl-.alpha.-carboline, m. 227-9.degree. (5:1 iso-PrOH-MeOCH2CH2OH). BuNH2 (7.5 ml) and 2 g 2-chloro-6-(N-methylanilino)-5-nitropyridine refluxed 30 min gave 2-(butylamino)-6-(N-methylanilino)-5-nitropyridine, m. 93-9.degree. (alc.), reduced catalytically over prerduced PtO2 and acidified to give 3-amino-6-butylamino-2-(N-methylanilino)pyridine-2-HBr, m. 170-92.degree. (decompn.). The base diazotized, heated with Cu powder at 30.degree. and the product analyzed chromatographically showed the presence of I (R = Me, X = BuNH). The compds. present a pronounced antiviral activity against herpes simplex, adenovirus SV 17, influenza A2, parainfluenza I, rhinovirus type I, rhinovirus type V and virus Coxsackie A 21, and show a surprising lack of toxicity on oral or subcutaneous administration. I (R = Me2N(CH2)3, X = Cl, shows neuroleptic activity.

ST antiviral neuroleptic carbolines; neuroleptic antiviral carbolines;  
carbolines antiviral neuroleptic

IT Virucides

(pyridoindole derivs.)

IT	6604-76-8P	25208-09-7P	25433-25-4P	26066-77-3P	26148-33-4P
	26148-34-5P	<b>26148-35-6P</b>	26148-36-7P	26148-37-8P	
	26148-59-4P	26148-60-7P	26148-61-8P	26148-66-3P	26148-67-4P
	26148-68-5P	26148-70-9P	26148-71-0P	26148-72-1P	26148-73-2P
	26148-74-3P	26148-75-4P	26259-75-6P	26866-91-1P	26866-92-2P
	26866-93-3P	26866-94-4P	26866-95-5P	26866-96-6P	26866-97-7P
	26866-98-8P	26866-99-9P	26867-00-5P	26867-01-6P	26867-02-7P
	26867-03-8P	26867-04-9P	26867-05-0P	26867-06-1P	26867-07-2P
	26867-08-3P	26867-09-4P	26867-10-7P	26867-11-8P	26867-12-9P
	26867-13-0P	26867-15-2P	26867-18-5P	26867-19-6P	26867-20-9P
	26867-21-0P	26867-22-1P	26867-23-2P	26867-24-3P	26867-25-4P
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	26869-20-5P	26869-21-6P	26869-22-7P	26869-23-8P	26869-24-9P
	26869-25-0P	26869-26-1P	26869-27-2P	26869-28-3P	26869-30-7P
	26942-46-1P	26942-49-4P	27183-68-2P		

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)



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=> S 26148-35-6/RN

L18 1 26148-35-6/RN

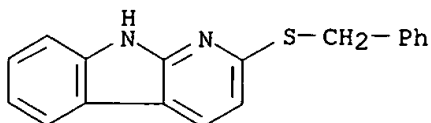
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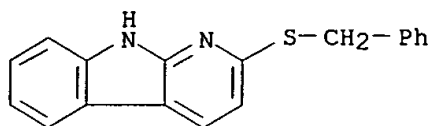
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CN 9H-Pyrido[2,3-b]indole, 2-(benzylthio)- (8CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C18 H14 N2 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER  
(\*File contains numerically searchable property data)





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2 REFERENCES IN FILE CA (1907 TO DATE)  
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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4  
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> e antiviral

E1	6	ANTIVIR/BI
E2	1	ANTIVIRA/BI
E3	41240 -->	ANTIVIRAL/BI
E4	1	ANTIVIRALE/BI
E5	2	ANTIVIRALEN/BI
E6	103	ANTIVIRALLY/BI
E7	847	ANTIVIRALS/BI
E8	1	ANTIVIREMIC/BI

E9 111 ANTIVIRIAL/BI  
 E10 2 ANTIVIRIALS/BI  
 E11 1 ANTIVIRICALLY/BI  
 E12 1 ANTIVIRIL/BI

=> s e3-e9

41240 ANTIVIRAL/BI  
 1 ANTIVIRALE/BI  
 2 ANTIVIRALEN/BI  
 103 ANTIVIRALLY/BI  
 847 ANTIVIRALS/BI  
 1 ANTIVIREMIC/BI  
 111 ANTIVIRIAL/BI  
 L19 41468 (ANTIVIRAL/BI OR ANTIVIRALE/BI OR ANTIVIRALEN/BI OR ANTIVIRALLY/  
 BI OR ANTIVIRALS/BI OR ANTIVIREMIC/BI OR ANTIVIRIAL/BI)

=> s 119 and 111

L20 21 L19 AND L11

=> s 120 not 112

L21 15 L20 NOT L12

=> s 121 not 116

L22 13 L21 NOT L16

=> d 122 1-13

L22 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2004:2860 CAPLUS  
 TI Preparation of 8-(biaryl)quinolines as PDE4 inhibitors  
 IN Deschenes, Denis; Dube, Daniel; Dube, Laurence; Gallant, Michel; Girard,  
 Yves; Lacombe, Patrick; MacDonald, Dwight  
 PA Merck Frosst Canada & Co., Can.  
 SO PCT Int. Appl., 122 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004000814	A1	20031231	WO 2003-CA957	20030623
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2002-391364P	P	20020625		
	US 2002-428313P	P	20021122		

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:980837 CAPLUS  
 DN 140:42459  
 TI Preparation of dimethylcyclobutane amino acid derivatives as prenylation  
 inhibitors

IN Brown, Bradley B.; Rehder, Kenneth S.; Strachan, Jon-Paul; Eaves, Jeron  
H.; Lowden, Christopher T.  
PA PPD Discovery, Inc., USA  
SO U.S., 24 pp., Cont.-in-part of U.S. Ser. No. 219,851, abandoned.  
CODEN: USXXAM  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6664277	B1	20031216	US 2003-336186	20030103
PRAI	US 2002-219851	B2	20020814		

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2003:913155 CAPLUS  
DN 139:391329  
TI Pyranone inhibitors of hepatitis C virus RNA-dependent RNA polymerase, and  
compositions and treatments using the same  
IN Gonzalez, Javier; Borchardt, Allen John; Dragovich, Peter Scott; Jewell,  
Tanya Michelle; Linton, Maria Angelica; Zhou, Ru; Li, Hui; Tatlock, John  
Howard; Abreo, Melwyn A.; Prins, Thomas J.  
PA Pfizer Inc., USA; et al.  
SO PCT Int. Appl., 269 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003095441	A1	20031120	WO 2003-IB1905	20030507
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRAI	US 2002-379433P	P	20020510		
OS	MARPAT 139:391329				

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2003:757679 CAPLUS  
DN 139:276825  
TI Preparation of 8-arylquinoline PDE4 inhibitors  
IN Gallant, Michel; Lacombe, Patrick; Dube, Daniel; Deschenes, Denis;  
MacDonald, Dwight; Dube, Laurence  
PA Merck Frosst Canada & Co., Can.  
SO PCT Int. Appl., 184 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI WO 2003078397 A1 20030925 WO 2003-CA374 20030317  
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
PRAI US 2002-365088P P 20020318  
OS MARPAT 139:276825  
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:504649 CAPLUS  
DN 137:83638  
TI Concomitant drugs of p38MAP kinase inhibitors and/or TNF-.alpha. prodn. inhibitors with other specified agents  
IN Ohkawa, Shigenori; Naruo, Kenichi; Miwatashi, Seiji  
PA Takeda Chemical Industries, Ltd., Japan  
SO PCT Int. Appl., 278 pp.  
CODEN: PIXXD2  
DT Patent  
LA Japanese  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002051442	A1	20020704	WO 2001-JP11353	20011225
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	JP 2002302458	A2	20021018	JP 2001-392778	20011225
	EP 1354603	A1	20031022	EP 2001-271876	20011225
	R:				
	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	JP 2000-396220	A	20001226		
	JP 2001-27572	A	20010202		
	WO 2001-JP11353	W	20011225		
OS	MARPAT 137:83638				
RE.CNT	58				
	THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD				
	ALL CITATIONS AVAILABLE IN THE RE FORMAT				

L22 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:256041 CAPLUS  
DN 136:294826  
TI Preparation of benzimidazolone **antiviral** agents  
IN Yu, Kuo-Long; Civiello, Rita; Combrink, Keith; Gulgeze, Hatice Belgin; Pearce, Bradley C.; Wang, Xiangdong; Meanwell, Nicholas A.; Zhang, Yi  
PA Bristol-Myers Squibb Company, USA  
SO PCT Int. Appl., 216 pp.  
CODEN: PIXXD2  
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002026228	A1	20020404	WO 2001-US29493	20010927
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 6506738	B1	20030114	US 2001-952736	20010914

PRAI US 2000-235804P P 20000927

OS MARPAT 136:294826

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:10451 CAPLUS

DN 136:85837

TI Preparation of benzodiazepines as inhibitors of HPV E1 helicase

IN Hurst, David Nigel; Jones, Philip Stephen; Parkes, Kevin Edward Burdon; Parratt, Martin John; Wilson, Francis Xavier

PA F. Hoffmann-La Roche A.-G., Switz.

SO PCT Int. Appl., 119 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002000632	A1	20020103	WO 2001-EP6895	20010619
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	EP 1299364	A1	20030409	EP 2001-949420	20010619
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
	US 2002128262	A1	20020912	US 2001-892148	20010626
PRAI	GB 2000-15904	A	20000628		
	WO 2001-EP6895	W	20010619		

OS MARPAT 136:85837

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:31464 CAPLUS

DN 134:100762

TI Preparation of pyridine derivatives and medicinal use thereof

IN Iino, Yukio; Fujita, Kohichi; Kodaira, Ariko; Hatanaka, Toshihiro;

Takehana, Kenji; Kobayashi, Tsuyoshi; Konishi, Atsushi; Yamamoto, Takashi

PA Ajinomoto Co., Inc., Japan

SO PCT Int. Appl., 86 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002359	A1	20010111	WO 2000-JP4298	20000629
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	EP 1193255	A1	20020403	EP 2000-940879	20000629
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
	BR 2000012046	A	20020514	BR 2000-12046	20000629
	TW 519538	B	20030201	TW 2000-89113050	20000630
	US 2002133005	A1	20020919	US 2001-29871	20011231
PRAI	JP 1999-187959	A	19990701		
	JP 2000-71706	A	20000315		
	WO 2000-JP4298	W	20000629		

OS MARPAT 134:100762

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:772628 CAPLUS

DN 133:321879

TI Preparation of 5-pyridyl-1,3-azole compounds as antagonists of adenosine A3 receptor, process for producing the same and use thereof

IN Ohkawa, Shigenori; Kanzaki, Naoyuki; Miwatashi, Seiji

PA Takeda Chemical Industries, Ltd., Japan

SO PCT Int. Appl., 152 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000064894	A1	20001102	WO 2000-JP2575	20000420
	W:	AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	EP 1180518	A1	20020220	EP 2000-917375	20000420
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
	BR 2000009952	A	20020326	BR 2000-9952	20000420
	NZ 515215	A	20030725	NZ 2000-515215	20000420
	AU 765473	B2	20030918	AU 2000-38401	20000420
	JP 2001114779	A2	20010424	JP 2000-126289	20000421
	JP 3333774	B2	20021015		
	JP 2002363179	A2	20021218	JP 2002-164744	20000421
	NO 2001005156	A	20011218	NO 2001-5156	20011022

ZA 2001008996      A      20030131      ZA 2001-8996      20011031  
 PRAI JP 1999-116686      A      19990423  
       JP 1999-224650      A      19990806  
       WO 2000-JP2575      W      20000420  
       JP 2000-126289      A3      20000421

OS MARPAT 133:321879

RE.CNT 20      THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD  
                  ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1996:155490 CAPLUS

DN 124:202255

TI Preparation of sulfur-containing heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents

IN Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil, Clara I.

PA G. D. Searle and Co., USA

SO PCT Int. Appl., 212 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9529897	A1	19951109	WO 1995-US5021	19950501
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9523950	A1	19951129	AU 1995-23950	19950501
	US 5945425	A	19990831	US 1996-737251	19961024
	US 2001047038	A1	20011129	US 2001-885221	20010620
PRAI	US 1994-235619	A2	19940429		
	WO 1995-US5021	W	19950501		
	US 1996-659098	B1	19960604		
	US 1999-377888	B1	19990819		
	US 2000-605560	B1	20000627		

OS MARPAT 124:202255

L22 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1993:539204 CAPLUS

DN 119:139204

TI Preparation of 5-halothiazetoquinoline-3-carboxylic acid derivatives as antibacterial, antitumor, and anti-AIDS virus agents

IN Ito, Yasuo; Kato, Hideo; Yasuda, Shingo; Yoshida, Toshihiko; Yamamoto, Yoichi

PA Hokuriku Pharmaceutical, Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05059067	A2	19930309	JP 1991-252762	19910905
PRAI	JP 1991-252762		19910905		

OS MARPAT 119:139204

L22 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN



AN 1987:32855 CAPLUS  
 DN 106:32855  
 TI 2,5-Bis(alkylsulfonyl)- and 2,5-bis(alkylthio)-substituted-pyridines  
 IN Wood, Steven G.  
 PA Dow Chemical Co., USA  
 SO U.S., 9 pp.  
 CODEN: USXXAM

DT Patent  
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4616087	A	19861007	US 1982-380642	19820521
PRAI	US 1982-380642		19820521		
OS	CASREACT 106:32855				

L22 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1983:155211 CAPLUS

DN 98:155211

TI Sulfur-substituted phenoxypyridines having **antiviral** activity

IN Markley, Lowell D.; Tong, Yulan C.; Wood, Steven G.

PA Dow Chemical Co., USA

SO U.S., 22 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4371537	A	19830201	US 1981-292467	19810813
	ZA 8205762	A	19830629	ZA 1982-5762	19820809
	IL 66496	A1	19851129	IL 1982-66496	19820809
	CA 1180017	A1	19841225	CA 1982-409151	19820810
	EP 72529	A1	19830223	EP 1982-107263	19820811
	EP 72529	B1	19860129		
	R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
	GB 2103619	A1	19830223	GB 1982-23098	19820811
	GB 2103619	B2	19850227		
	AU 8287078	A1	19830512	AU 1982-87078	19820811
	AU 551683	B2	19860508		
	AT 17719	E	19860215	AT 1982-107263	19820811
	NO 8202751	A	19830214	NO 1982-2751	19820812
	NO 159851	B	19881107		
	NO 159851	C	19890215		
	DK 8203628	A	19830214	DK 1982-3628	19820812
	DK 157297	B	19891204		
	DK 157297	C	19900507		
	JP 58041868	A2	19830311	JP 1982-139277	19820812
	JP 04014107	B4	19920311		
	ES 514940	A1	19831016	ES 1982-514940	19820812
	ES 523661	A1	19850316	ES 1983-523661	19830628
	ES 523660	A1	19850401	ES 1983-523660	19830628
PRAI	US 1981-292467		19810813		
	EP 1982-107263		19820811		
OS	CASREACT 98:155211				

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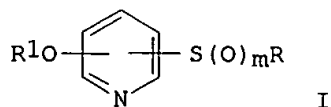
L22 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1983:155211 CAPLUS

DN 98:155211

ED Entered STN: 12 May 1984  
 TI Sulfur-substituted phenoxypyridines having **antiviral** activity  
 IN Markley, Lowell D.; Tong, Yulan C.; Wood, Steven G.  
 PA Dow Chemical Co., USA  
 SO U.S., 22 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC A61K031-44; C07D021-263  
 NCL 424263000  
 CC 1-5 (Pharmacology)  
 Section cross-reference(s): 27  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4371537	A	19830201	US 1981-292467	19810813
	ZA 8205762	A	19830629	ZA 1982-5762	19820809
	IL 66496	A1	19851129	IL 1982-66496	19820809
	CA 1180017	A1	19841225	CA 1982-409151	19820810
	EP 72529	A1	19830223	EP 1982-107263	19820811
	EP 72529	B1	19860129		
	R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
	GB 2103619	A1	19830223	GB 1982-23098	19820811
	GB 2103619	B2	19850227		
	AU 8287078	A1	19830512	AU 1982-87078	19820811
	AU 551683	B2	19860508		
	AT 17719	E	19860215	AT 1982-107263	19820811
	NO 8202751	A	19830214	NO 1982-2751	19820812
	NO 159851	B	19881107		
	NO 159851	C	19890215		
	DK 8203628	A	19830214	DK 1982-3628	19820812
	DK 157297	B	19891204		
	DK 157297	C	19900507		
	JP 58041868	A2	19830311	JP 1982-139277	19820812
	JP 04014107	B4	19920311		
	ES 514940	A1	19831016	ES 1982-514940	19820812
	ES 523661	A1	19850316	ES 1983-523661	19830628
	ES 523660	A1	19850401	ES 1983-523660	19830628
PRAI	US 1981-292467		19810813		
	EP 1982-107263		19820811		
OS	CASREACT 98:155211				
GI					



AB The title compds. I [R = C1-7 alkyl, C5 or C6 cycloalkyl, Ar(CH<sub>2</sub>)<sub>q</sub> (Ar = C6-10 aryl, q = 0-3), R<sub>1</sub> = Ph or substituted Ph; m = 0, 1, or 2] preferably administered as pharmaceutical compns. (no data given) were prepd. by several methods and evaluated as **antiviral** agents. Thus, 2-(3,4-dichlorophenoxy)-5-(methylsulfonyl)pyridine [85331-30-2] prepd. by the reaction of 3,4-dichlorophenol [95-77-2] in DMSO in presence of Na tert-butoxide with 2,5-bis(methylsulfonyl)pyridine showed a broad spectrum **antiviral** activity at low conc. (25 .mu.g/mL).  
 ST phenoxythiopyridine prepn **antiviral**; virucide

phenoxythiopyridine; pyridine phenoxythio prepn **antiviral**

IT Virucides and Virustats  
(phenoxythiopyridines)

IT 85330-61-6P 85330-67-2P 85330-70-7P 85330-73-0P **85330-76-3P**  
85331-31-3P 85331-32-4P 85331-38-0P 85331-39-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and decarboxylation of)

IT 85331-36-8P 85331-37-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and hydrolysis of)

IT 58819-71-9P 71506-85-9P 85330-62-7P 85330-65-0P 85330-68-3P  
85330-69-4P 85330-71-8P 85330-74-1P **85330-77-4P**  
85330-81-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and oxidn. of)

IT 85331-34-6P 85331-35-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reaction with dichlorophenol)

IT 85330-72-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reaction with hydroxyacetophenone)

IT **85330-78-5P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reaction with hydroxybenzophenone)

IT 25935-30-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reaction with sodium methanethiolate)

IT 85330-63-8P 85330-64-9P 85330-66-1P 85330-75-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reaction with substituted phenols)

IT 25935-29-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and redn. of)

IT 85330-84-3P 85330-85-4P 85330-86-5P 85330-87-6P 85330-88-7P  
85330-89-8P 85330-90-1P 85330-91-2P 85330-92-3P 85330-93-4P  
85330-94-5P 85330-95-6P 85330-96-7P 85330-97-8P 85330-98-9P  
85330-99-0P 85331-00-6P 85331-01-7P 85331-02-8P 85331-03-9P  
85331-04-0P 85331-05-1P 85331-06-2P 85331-07-3P 85331-08-4P  
85331-09-5P 85331-10-8P 85331-11-9P 85331-12-0P 85331-13-1P  
85331-14-2P 85331-15-3P 85331-16-4P 85331-17-5P 85331-18-6P  
85331-19-7P 85331-20-0P 85331-21-1P 85331-22-2P 85331-23-3P  
85331-24-4P 85331-25-5P 85331-26-6P 85331-27-7P 85331-28-8P  
85331-29-9P 85331-30-2P 85345-64-8P 85368-98-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and virucidal activity)

IT 62916-42-1P 85330-79-6P 85330-80-9P 85330-82-1P 85330-83-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

IT 75-33-2  
RL: BIOL (Biological study)  
(reaction of with Me dichloropyridinecarboxylate)

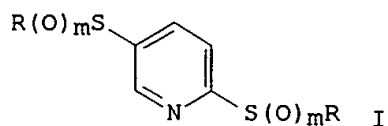
IT 100-53-8 108-98-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with Me dichloropyridinecarboxylate)  
 IT 95-95-4 533-31-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with bis(ethylsulfonyl)pyridine)  
 IT 98-54-4 99-93-4 101-53-1 106-41-2 106-48-9 461-84-7 591-20-8  
 767-00-0 831-82-3 873-62-1 1073-72-9 1137-42-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with bis(methylsulfonyl)pyridine)  
 IT 95-77-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with chloronitropyridine)  
 IT 140-89-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with diazotized pyridine derivs.)  
 IT 4548-45-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with dichlorophenol)  
 IT 1569-69-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with dichloropyridinecarboxylic acid)  
 IT 75-08-1 111-31-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with dichloropyridinecarboxylic acid)  
 IT 1532-24-7 1702-17-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with mercaptans)  
 IT 26452-80-2 85331-33-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with methanethiol)  
 IT 74-93-1, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with pyridinecarboxylates)

=> d 122 12 all

L22 .ANSWER 12 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1987:32855 CAPLUS  
 DN 106:32855  
 ED Entered STN: 07 Feb 1987  
 TI 2,5-Bis(alkylsulfonyl)- and 2,5-bis(alkylthio)-substituted-pyridines  
 IN Wood, Steven G.  
 PA Dow Chemical Co., USA  
 SO U.S., 9 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07D211-72  
 ICS C07D211-84  
 NCL 546294000  
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 1  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4616087	A	19861007	US 1982-380642	19820521
PRAI	US 1982-380642		19820521		
OS	CASREACT 106:32855				
GI					



- AB The title compds. I (R = C1-7 alkyl, cycloalkyl, Ar(CH<sub>2</sub>)<sub>q</sub>, Ar = (un)substituted Ph, naphthyl; q = 0-3; m = 0-2) useful as **antiviral** agents, were prepd. Thus, to 4-F<sub>3</sub>CSC<sub>6</sub>H<sub>4</sub>OH in THF was added Me<sub>3</sub>COK and 2,5-bis(methylsulfonyl)pyridine, prepd. in 3 steps from Me 3,6-dichloro-2-pyridinecarboxylate, to give 5-(methylsulfonyl)-2-[4-[(trifluoromethyl)thio]phenoxy]pyridine (II). II at 12.5 .mu.g/mL was active against rhinovirus type 1A.
- ST pyridine alkylsulfonyl phenoxy prepn **antiviral**
- IT Virucides and Virustats  
(bis(alkylsulfonyl)- and bis(alkylthio)-substituted-pyridines)
- IT 533-31-3, 3,4-(Methylenedioxy)phenol  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with bis(ethylsulfonyl)pyridine)
- IT 106-41-2, 4-Bromophenol  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with bis(hexylsulfonyl)pyridine)
- IT 461-84-7, 4-(Trifluoromethylthio)phenol  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with bis(methylsulfonyl)pyridine)
- IT 95-77-2, 3,4-Dichlorophenol 99-93-4, p-Hydroxyacetophenone 1137-42-4, p-Hydroxybenzophenone  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with sulfonylpyridines)
- IT 85330-64-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with (methylenedioxy)phenol)
- IT 85330-63-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with (trifluoromethylthio)phenol)
- IT 85330-69-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with bromophenol)
- IT 85330-66-1P 85330-75-2P 85330-79-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with dichlorophenol)
- IT 85330-72-9P 85330-82-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with hydroxyacetophenone)
- IT **85330-78-5P** 85330-89-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with hydroxybenzophenone)
- IT 85330-61-6P 85330-67-2P 85330-70-7P 85330-73-0P **85330-76-3P**  
85331-32-4P 91164-62-4P 106025-37-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and decarboxylation of)
- IT 85331-31-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and decarboxylation-oxidn. of)
- IT 69212-36-8P 85330-62-7P 85330-65-0P 85330-68-3P 85330-71-8P  
85330-74-1P **85330-77-4P** 85330-80-9P 85330-81-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and oxidn. of)

IT 98626-97-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

IT 85330-84-3P 85330-85-4P 85330-86-5P 85330-87-6P 85330-88-7P  
 85330-90-1P 85330-91-2P 85330-92-3P 85330-93-4P 85330-96-7P  
 85330-97-8P 85330-98-9P 85330-99-0P 85331-02-8P 85331-03-9P  
 85331-04-0P 85331-05-1P 85331-06-2P 85331-07-3P 85331-08-4P  
 85331-09-5P 85331-10-8P 85331-11-9P 85331-12-0P 85331-13-1P  
 85331-14-2P 85331-15-3P 85331-16-4P 85331-17-5P 85331-18-6P  
 85331-25-5P 85331-26-6P 85331-27-7P 85331-28-8P 85345-64-8P  
 85368-98-5P 99902-97-3P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
 BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of, as virucide)

IT 74-93-1, reactions 75-33-2 111-31-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (substitution by, of Me dichloropyridinecarboxylate)

IT 75-08-1 100-53-8, Benzyl mercaptan 108-98-5, Thiophenol, reactions  
 1569-69-3, Cyclohexyl mercaptan  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (substitution by, of dichloropyridinecarboxylic acid)

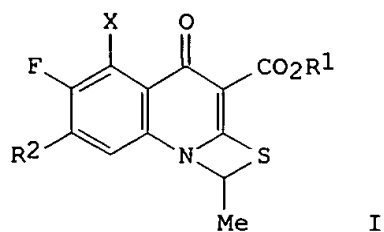
IT 1702-17-6, 3,6-Dichloro-2-pyridinecarboxylic acid 88912-24-7,  
 5,6-Dichloro-2-pyridinecarboxylic acid  
 RL: PROC (Process)  
 (substitution of, with mercaptans)

IT 1532-24-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (substitution with alkanethiol and hydrolysis of)

=> d 122 11 all

L22 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1993:539204 CAPLUS  
 DN 119:139204  
 ED Entered STN: 02 Oct 1993  
 TI Preparation of 5-halothiazetoquinoline-3-carboxylic acid derivatives as  
 antibacterial, antitumor, and anti-AIDS virus agents  
 IN Ito, Yasuo; Kato, Hideo; Yasuda, Shingo; Yoshida, Toshihiko; Yamamoto,  
 Yoichi  
 PA Hokuriku Pharmaceutical, Japan  
 SO Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC ICM C07D513-04  
 ICS A61K031-47  
 CC 28-4 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	JP 05059067	A2	19930309	JP 1991-252762	19910905
PRAI	JP 1991-252762		19910905		
OS	MARPAT 119:139204				
GI					



- AB The title derivs. I [R1 = H, lower alkyl; R2 = halo, (un)substituted cyclic amino; X = halo) and their pharmaceutically acceptable salts, useful as bactericides, neoplasm inhibitors, and anti-AIDS virus agents (no data), are claimed. A DMF soln. of 16.0 g 5-chloro-6,7-difluoro-1,2-dihydro-4-hydroxy-2-thioxo-3-quinolinecarboxylic acid Et ester (prepn. given) was added dropwise to a mixt. of MeCHI2, K2CO3, and DMF at 90-100.degree. over 40 min to give 9.52 g I (R1 = Et, R2 = F, X = Cl).
- ST thiazetoquinolinecarboxylate prepn antitumor antibacterial **antiviral**; AIDS virus inhibitor thiazetoquinolinecarboxylate prepn; neoplasm inhibitor thiazetoquinolinecarboxylic acid prepn; bactericide thiazetoquinolinecarboxylic acid prepn
- IT Bactericides, Disinfectants, and Antiseptics  
Neoplasm inhibitors  
(thiazetoquinolinecarboxylic acid derivs.)
- IT Acquired immune deficiency syndrome  
(thiazetoquinolinecarboxylic acid derivs. for treatment of)
- IT Virucides and Virustats  
(thiazetoquinolinecarboxylic acid derivs., for human immunodeficiency virus-1)
- IT Virus, animal  
(human immunodeficiency, thiazetoquinolinecarboxylic acid derivs. as inhibitors for)
- IT 64695-81-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination of)
- IT 149144-07-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and cyclization of, (benzylthio)quinolinecarboxylic acid deriv. from)
- IT 149144-09-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and cyclocondensation of, with diiodoethane, thiazetoquinoline deriv. from)
- IT 149144-04-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and deacetylation and debromination of)
- IT **149144-08-1P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and reaction of, thioxoquinoline deriv. from)
- IT 149636-28-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and reaction of, with Et chlorocarbonate, isothiocyanate from)
- IT 149144-05-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and reaction of, with carbon disulfide, dithiocarbamate from)

IT 149144-06-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and reaction of, with di-Et malonate and methoxybenzyl chloride, [anilino(benzylthio)methylene]malonate deriv. from)

IT 149144-10-5P 149144-11-6P 149144-12-7P 149636-30-6P 149665-60-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of, as antitumor and antibacterial and anti-AIDS virus agent)

IT 824-94-2, 4-Methoxybenzyl chloride  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with Ph isothiocyanate deriv. and di-Et malonate, [anilino(benzylthio)methylene]malonate deriv. from)

IT 105-53-3, Diethyl malonate  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with Ph isothiocyanate deriv. and methoxybenzyl chloride, [anilino(benzylthio)methylene]malonate deriv. from)

IT 132883-43-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with thiazetoquinoline deriv.)

=> d 122 10 all

L22 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1996:155490 CAPLUS  
 DN 124:202255  
 ED Entered STN: 19 Mar 1996  
 TI Preparation of sulfur-containing heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents  
 IN Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil, Clara I.  
 PA G. D. Searle and Co., USA  
 SO PCT Int. Appl., 212 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D235-28  
 ICS A61K031-415; C07D401-12; A61K031-44; C07D233-84  
 CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9529897	A1	19951109	WO 1995-US5021	19950501
	W:				
	AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW:				
	KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9523950	A1	19951129	AU 1995-23950	19950501
	US 5945425	A	19990831	US 1996-737251	19961024
	US 2001047038	A1	20011129	US 2001-885221	20010620
PRAI	US 1994-235619	A2	19940429		
	WO 1995-US5021	W	19950501		
	US 1996-659098	B1	19960604		
	US 1999-377888	B1	19990819		
	US 2000-605560	B1	20000627		

OS MARPAT 124:202255

AB The title compds., which are (H+/K+) ATPase inhibitors, useful for the treatment of viral infections, are prepd. and formulations contg. them are



claimed. Thus, 2-[(1H-benzimidazol-2-yl)sulfinylmethyl]-N,N-dimethylbenzenamine, m.p. 107-109.degree., was prepd. and demonstrated a (H+/K+) ATPase IC50 of 0.7 .mu.M.

ST benzimidazolylsulfinylmethylmethylbenzenamine prepn ATPase inhibitor;  
antiviral agent prepn benzimidazolylsulfinylmethylmethylbenzenamine;  
benzimidazolyl sulfinylmethylmethylbenzenamine

IT Ulcer inhibitors

Virucides and Virustats

(heterocyclic (H+/K+) ATPase inhibitors)

IT 9000-83-3, ATPase

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(potassium-hydrogen-activated; prepn. of sulfur-contg. heterocyclic

(H+/K+) ATPase inhibitors as **antiviral** agents)

IT	55546-06-0P	56713-45-2P	57235-18-4P	60524-97-2P	71670-48-9P
	73590-36-0P	73590-58-6P	73590-61-1P	81527-04-0P	81864-40-6P
	81864-65-5P	94452-40-1P	96733-60-7P	97288-52-3P	97963-93-4P
	97966-85-3P	98412-35-2P	98412-41-0P	99153-80-7P	99153-89-6P
	99499-40-8P	100924-68-3P	101387-98-8P	102127-07-1P	102127-11-7P
	102625-70-7P	102625-79-6P	103014-24-0P	103577-45-3P	103922-27-6P
	103971-24-0P	104340-33-2P	104340-34-3P	104340-35-4P	104340-37-6P
	104340-38-7P	104340-41-2P	104340-86-5P	104524-67-6P	104524-68-7P
	104658-07-3P	104685-57-6P	104987-90-8P	105389-48-8P	105950-65-0P
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	106785-96-0P	106850-06-0P	107512-17-4P	108026-58-0P	108499-76-9P
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	111476-84-7P	111476-85-8P	111476-86-9P	111476-87-0P	111476-88-1P
	111476-89-2P	111476-91-6P	111476-92-7P	111476-93-8P	111476-94-9P
	111476-95-0P	111476-96-1P	111476-97-2P	111476-98-3P	111476-99-4P
	111477-01-1P	111477-02-2P	111477-03-3P	111477-04-4P	111477-14-6P
	111502-75-1P	111604-57-0P	111858-83-4P	112058-72-7P	112058-73-8P
	112230-13-4P	112645-53-1P	112705-43-8P	113418-90-9P	113703-12-1P
	113703-14-3P	113703-21-2P	113703-22-3P	113703-28-9P	113712-97-3P
	113805-04-2P	113855-38-2P	113855-39-3P	113855-40-6P	113855-41-7P
	113855-42-8P	113915-02-9P	113942-61-3P	114060-19-4P	114560-55-3P
	115046-03-2P	115366-78-4P	115366-80-8P	116091-77-1P	116940-41-1P
	117038-05-8P	117046-87-4P	117347-86-1P	117426-11-6P	117934-10-8P
	117977-41-0P	118267-21-3P	118267-22-4P	118267-23-5P	118267-24-6P
	118267-25-7P	118267-26-8P	118267-27-9P	118267-28-0P	118267-29-1P
	118267-30-4P	118267-31-5P	118267-32-6P	118267-33-7P	118267-34-8P
	118267-35-9P	118267-36-0P	118267-37-1P	118267-38-2P	118267-39-3P
	118267-42-8P	118267-43-9P	118292-92-5P	118292-93-6P	118292-94-7P
	118292-95-8P	118292-96-9P	118292-97-0P	118292-98-1P	118292-99-2P
	120009-37-2P	120393-57-9P	120699-85-6P	120699-91-4P	120894-65-7P
	121050-40-6P	121242-64-6P	121591-86-4P	122223-85-2P	122307-32-8P
	122508-81-0P	123215-59-8P	123215-83-8P	123451-58-1P	123823-95-0P
	123907-70-0P	123987-02-0P	124736-45-4P	124899-76-9P	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as antiviral agents)

IT	125214-42-8P	126026-46-8P	128429-74-3P	128935-96-6P	128936-05-0P
	130049-59-1P	130368-60-4P	130368-62-6P	130368-66-0P	133903-90-9P
	134017-66-6P	134462-81-0P	135430-38-5P	135461-65-3P	135863-25-1P
	137105-02-3P	137247-56-4P	137810-46-9P	139644-93-2P	139767-99-0P
	142062-72-4P	150064-18-9P	150460-06-3P	153284-85-6P	174397-92-3P
	174397-93-4P	174397-94-5P	174397-95-6P	174397-96-7P	174397-97-8P
	174397-98-9P	174397-99-0P	174398-00-6P	174398-01-7P	174398-02-8P
	174398-03-9P	174398-04-0P	174398-05-1P	174398-06-2P	
	174398-07-3P	174398-08-4P	174398-09-5P	174398-10-8P	174398-11-9P
	174398-12-0P	174398-13-1P	174398-14-2P	174398-15-3P	174398-16-4P
	174398-17-5P	174398-18-6P	174398-19-7P	174398-20-0P	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as antiviral agents)

IT 144114-21-6, Retropepsin

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as antiviral agents)

IT	85-44-9, Phthalic anhydride	94-09-7, Ethyl 4-aminobenzoate	110-18-9
	140-89-6, Potassium ethylxanthate	400-98-6, 4-(Trifluoromethyl)-2-nitroaniline	446-33-3, 3-Fluoro-6-nitrotoluene
	455-14-1, 4-(Trifluoromethyl)aniline	583-39-1, 2-Mercaptobenzimidazole	1603-41-4, 2-Amino-5-methylpyridine
	1635-61-6, 3-Chloro-6-nitroaniline	1635-84-3, 2,4-Dimethyl-6-nitroaniline	1639-31-2, 3,4,5-Trimethylaniline
	1824-81-3, 2-Amino-6-methylpyridine	2127-03-9, 2,2'-Dipyridyl disulfide	3171-45-7, 4,5-Dimethyl-1,2-phenylenediamine
	3287-79-4, 2-Mercapto-5,6-dimethylbenzimidazole	5327-33-3, 2-Acetamido-6-methylpyridine	5344-90-1, 2-Aminobenzyl alcohol
	7595-31-5, 25369-78-2	27231-33-0, 2-Mercapto-4-methylbenzimidazole	27231-36-3, 27492-84-8,
	Methyl 4-amino-2-methoxybenzoate	30525-89-4, Paraformaldehyde	37052-78-1, 2-Mercapto-5-methoxybenzimidazole
	39785-37-0, 4-Methoxy-3,5-dimethylaniline	55489-15-1, 71675-52-0,	2-(Bromomethyl)-4-chloroaniline hydrobromide
	71693-08-8, 2-(Bromomethyl)-5-chloroaniline hydrobromide	74004-74-3, 86604-73-1	88301-76-2, 88301-77-3, 88301-78-4, 88301-79-5, 88301-81-9,
	2-(Chloromethyl)aniline hydrochloride	90562-37-1, N-[2-(Chloromethyl)phenyl]acetamide	92333-53-4, 92643-51-1, 92807-01-7
	106746-59-2, 2-(Chloromethyl)-4-methoxyaniline hydrochloride	106746-62-7	106746-64-9, 106746-67-2, 106746-71-8, 106746-85-4, 106746-87-6
	106746-89-8, 106746-91-2, 106746-92-3, 106746-99-0, 106771-59-9,	2-(Chloromethyl)-N,N-dimethylaniline	174397-86-5, 174397-87-6
	174397-88-7		

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as antiviral agents)

IT	4093-29-2P, Methyl 4-acetamido-2-methoxybenzoate	25617-34-9P
	27841-33-4P, 59338-85-1P, Methyl 4,5-diamino-2-methoxybenzoate	
	86847-79-2P, 104524-65-4P, 106746-72-9P, 106746-73-0P, 106746-74-1P	
	106746-75-2P, 106746-81-0P, 106746-82-1P, 106746-83-2P, 106747-02-8P	
	106747-03-9P, 106747-04-0P, 106747-46-0P, 106771-57-7P, 118267-40-6P	
	165685-25-6P, 174397-89-8P, 174397-90-1P, 174397-91-2P, 174398-21-1P	
	174398-22-2P	

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

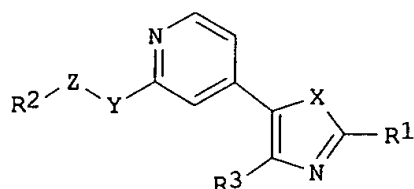
(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as

antiviral agents)

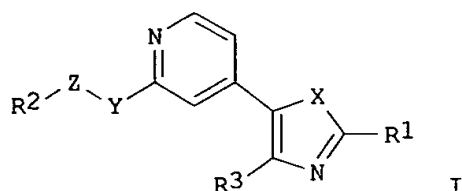
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L22 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2000:772628 CAPLUS  
 DN 133:321879  
 ED Entered STN: 03 Nov 2000  
 TI Preparation of 5-pyridyl-1,3-azole compounds as antagonists of adenosine  
 A3 receptor, process for producing the same and use thereof  
 IN Ohkawa, Shigenori; Kanzaki, Naoyuki; Miwatashi, Seiji  
 PA Takeda Chemical Industries, Ltd., Japan  
 SO PCT Int. Appl., 152 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA Japanese  
 IC ICM C07D417-04  
 ICS C07D417-14; A61K031-4439; A61P043-00; A61P029-00; A61P031-12;  
 A61P003-10; A61P001-00; A61P009-00; A61P007-00  
 CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 7  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000064894	A1	20001102	WO 2000-JP2575	20000420
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	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1180518	A1	20020220	EP 2000-917375	20000420
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	BR 2000009952	A	20020326	BR 2000-9952	20000420
	NZ 515215	A	20030725	NZ 2000-515215	20000420
	AU 765473	B2	20030918	AU 2000-38401	20000420
	JP 2001114779	A2	20010424	JP 2000-126289	20000421
	JP 3333774	B2	20021015		
	JP 2002363179	A2	20021218	JP 2002-164744	20000421
	NO 2001005156	A	20011218	NO 2001-5156	20011022
	ZA 2001008996	A	20030131	ZA 2001-8996	20011031
PRAI	JP 1999-116686	A	19990423		
	JP 1999-224650	A	19990806		
	WO 2000-JP2575	W	20000420		
	JP 2000-126289	A3	20000421		
OS	MARPAT 133:321879				
GI					



I



- AB Optionally N-oxidized compds. represented by general formula (I) salts thereof [wherein R1 represents hydrogen, hydrocarbyl, a heterocycle, amino or acyl; R2 represents an arom. group; R3 represents hydrogen, pyridyl or arom. hydrocarbyl; X represents oxygen or optionally oxidized sulfur; Y represents a bond, oxygen, optionally oxidized sulfur or NR4 (wherein R4 represents hydrogen, hydrocarbyl, or acyl); and Z represents a bond or a divalent chain hydrocarbyl] are prepd. These compds. are usable as preventives or remedies for diseases in assocn. with adenosine A3 receptor because of having excellent adenosine A3 receptor antagonism thereof. Moreover, the compds. I or salts thereof exhibit excellent effects of inhibiting p38 MAP kinase and inhibiting TNF-.alpha. and, therefore, are also usable as preventives or remedies for diseases in assocn. with p38 MAP kinase or TNF-.alpha.. Above diseases include asthma, allergies, brain edema, cerebral vascular disorders, head injuries, inflammation, Addison's disease, autoimmune hemolytic anemia, Crohn's disease, psoriasis, rheumatism, spinal cord injury, multiple sclerosis, Alzheimer's disease, Parkinson's disease, amyotrophic lateral sclerosis, diabetes, arthritis, septicemia, ulcerative colitis, chronic pneumonia, silicosis, lung sarcoidosis, pulmonary tuberculosis, cachexia, arteriosclerosis, Creutzfeldt-Jakob disease, virus infection, atopic dermatitis, systemic lupus erythematosus, AIDS encephalopathy, meningitis, angina pectoris, myocardial infarction, ischemic heart failure, hepatitis, transplant, dialysis hypotension, and frequent disseminated intravascular coagulation. Thus, bromination of 2-(2-benzoylamino-4-pyridyl)-1-(4-methoxyphenyl)ethanone with Br in AcOH at room temp. for 1 h followed by cyclocondensation of the bromination product with thiourea in the presence of Et3N in MeCN at 80.degree. for 5 h gave N-[4-[2-amino-4-(4-methoxyphenyl)-1,3-thiazol-5-yl]-2-pyridyl]benzamide (II). II showed IC50 of 0.020 .mu.M against p38 MAP kinase and 0.014 .mu.M for inhibiting the prodn. of TNF-.alpha. in THP-1 cells.
- ST pyridylazole prepn antagonist adenosine A3 receptor; pyridylthiazole prepn TNF alpha inhibitor; p38 MAP kinase inhibitor pyridylthiazole
- IT Adenosine receptors  
 RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
 (A3; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Brain, disease  
 Prion diseases  
 (Creutzfeldt-Jakob; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Intestine, disease  
 (Crohn's; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Nervous system  
 (amyotrophic lateral sclerosis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)
- IT Heart, disease

(angina pectoris; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Dermatitis  
(atopic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease  
(cerebrovascular; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Pneumonia  
(chronic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Blood coagulation  
(disseminated intravascular, frequent; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease  
(edema; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease  
(failure, ischemic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Anemia (disease)  
(hemolytic, autoimmune; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease  
(in assocn. with AIDS; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Hypotension  
(in assocn. with dialysis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease  
(infarction; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Head  
Spinal cord  
(injury; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Addison's disease  
Allergy inhibitors  
Alzheimer's disease  
Anti-inflammatory agents  
Antiarteriosclerotics  
Antiarthritics  
Antiasthmatics  
Antidiabetic agents  
Antirheumatic agents  
**Antiviral agents**  
Cachexia  
Hepatitis  
Meningitis  
Multiple sclerosis

Parkinson's disease

Psoriasis

Septicemia

Silicosis

Transplant and Transplantation

Tuberculosis

(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Tumor necrosis factors

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Lung, disease

(sarcoidosis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Lupus erythematosus

(systemic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Intestine, disease

(ulcerative colitis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 303162-57-4P 303162-71-2P 303162-72-3P 303162-74-5P 303162-75-6P

303162-76-7P 303162-77-8P 303162-78-9P 303162-79-0P 303162-80-3P

303162-85-8P 303162-86-9P 303162-87-0P 303162-88-1P 303162-89-2P

303162-90-5P 303162-91-6P 303162-92-7P 303162-93-8P 303162-94-9P

303162-95-0P 303162-96-1P 303163-15-7P 303163-17-9P 303163-18-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 303162-58-5P 303162-59-6P 303162-60-9P 303162-61-0P 303162-62-1P

303162-64-3P 303162-66-5P 303162-67-6P 303162-68-7P 303162-69-8P

303162-70-1P 303162-73-4P 303162-81-4P 303162-82-5P 303162-83-6P

303162-84-7P 303162-97-2P 303162-98-3P 303162-99-4P 303163-00-0P

303163-01-1P 303163-02-2P 303163-03-3P 303163-04-4P 303163-05-5P

303163-06-6P 303163-07-7P 303163-08-8P 303163-09-9P 303163-10-2P

303163-11-3P 303163-12-4P 303163-13-5P 303163-14-6P 303163-16-8P

303163-19-1P 303163-20-4P 303163-21-5P 303163-22-6P 303163-23-7P

303163-24-8P 303163-25-9P 303163-26-0P 303163-27-1P 303163-28-2P

303163-29-3P 303163-30-6P 303163-31-7P 303163-32-8P 303163-33-9P

303163-34-0P 303163-35-1P 303163-36-2P 303163-37-3P 303163-38-4P

303163-39-5P 303163-40-8P 303163-41-9P 303163-42-0P

**303163-43-1P** 303163-44-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 165245-96-5, p38 MAP kinase

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 62-55-5, Thioacetamide 62-56-6, Thiourea, reactions 64-04-0,  
2-Phenylethylamine 74-88-4, Methyl iodide, reactions 75-36-5, Acetyl  
chloride 75-55-8 98-88-4, Benzoyl chloride 100-07-2,

4-Methoxybenzoyl chloride 100-46-9, Benzylamine, reactions 100-51-6, Benzenemethanol, reactions 100-53-8, Phenylmethanethiol 103-67-3, N-Benzyl-N-methylamine 103-80-0, Phenylacetyl chloride 104-86-9, 4-Chlorobenzylamine 108-98-5, Thiophenol, reactions 109-74-0, Butyronitrile 110-59-8, Valeronitrile 140-75-0, 4-Fluorobenzylamine 499-06-9, 3,5-Dimethylbenzoic acid 589-08-2, N-Methyl-2-phenylethylamine 598-52-7, N-Methylthiourea 631-58-3, Thiopropionamide 645-45-4, 3-Phenylpropionyl chloride 772-70-3, 3-(4-Fluorophenyl)propionyl chloride 873-32-5, 2-Chlorobenzonitrile 1194-02-1, 4-Fluorobenzonitrile 1711-05-3, 3-Methoxybenzoyl chloride 1711-06-4, 3-Methylbenzoyl chloride 2243-83-6, 2-Naphthoyl chloride 2393-23-9, 4-Methoxybenzylamine 2627-86-3, (S)-1-Phenylethylamine 3886-69-9, (R)-1-Phenylethylamine 4152-90-3, 3-Chlorobenzylamine 4926-28-7, 2-Bromo-4-methylpyridine 5071-96-5, 3-Methoxybenzylamine 5271-67-0, 2-Thiophenecarbonyl chloride 6850-57-3, 2-Methoxybenzylamine 15893-42-2, 3-(4-Methoxyphenyl)propionyl chloride 18496-54-3, 4-Phenylbutyryl chloride 20260-53-1, Nicotinoyl chloride hydrochloride 20371-41-9, 5-Phenylvaleryl chloride 21382-98-9, 4-Methylthiobenzonitrile 27757-85-3, 2-Thienylmethylamine 90101-20-5, 2-(tert-Butoxycarbonylamino)-4-methylpyridine  
 RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)  
 IT 461-87-0P, 2-Fluoro-4-methylpyridine 6613-44-1P, 3,5-Dimethylbenzoyl chloride 15717-17-6P, 2-Chlorothiobenzamide 16536-93-9P, Thiobutyramide 16536-94-0P, Thiovaleramide 21384-43-0P 22179-72-2P, 4-Fluorothiobenzamide 53550-91-7P, 4-(Methylthio)thiobenzamide 102336-06-1P 224040-60-2P 224040-71-5P 303162-27-8P 303162-28-9P 303162-29-0P 303162-30-3P 303162-31-4P 303162-32-5P 303162-33-6P 303162-34-7P 303162-35-8P 303162-36-9P 303162-37-0P 303162-38-1P 303162-39-2P 303162-40-5P 303162-41-6P 303162-42-7P 303162-43-8P 303162-44-9P 303162-45-0P 303162-46-1P 303162-47-2P 303162-48-3P 303162-49-4P 303162-50-7P 303162-52-9P 303162-54-1P 303162-55-2P 303162-56-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD

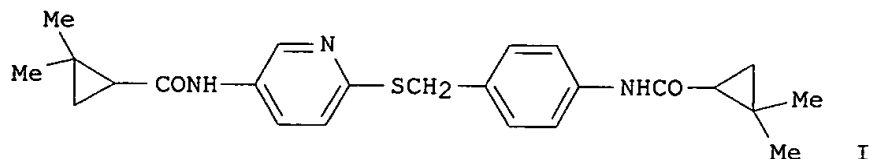
RE

- (1) Merck & Co Inc; JP 11514353 A
- (2) Merck & Co Inc; CN 1203590 A CAPLUS
- (3) Merck & Co Inc; NZ 321738 A
- (4) Merck & Co Inc; US 5717100 A CAPLUS
- (5) Merck & Co Inc; EP 854870 A1 CAPLUS
- (6) Merck & Co Inc; AU 9675143 A CAPLUS
- (7) Merck & Co Inc; SK 9800435 A
- (8) Merck & Co Inc; CZ 9801043 A
- (9) Merck & Co Inc; NO 9801528 A CAPLUS
- (10) Merck & Co Inc; HU 9902294 A
- (11) Merck & Co Inc; WO 9712876 A1 1997 CAPLUS
- (12) Otsuka Pharmaceutical Co Ltd; JP 10152437 A CAPLUS
- (13) Otsuka Pharmaceutical Co Ltd; CN 1232396 A CAPLUS
- (14) Otsuka Pharmaceutical Co Ltd; EP 957915 A1 CAPLUS
- (15) Otsuka Pharmaceutical Co Ltd; BR 9712140 A CAPLUS
- (16) Otsuka Pharmaceutical Co Ltd; AU 9743221 A CAPLUS
- (17) Otsuka Pharmaceutical Co Ltd; WO 9814191 A1 1998 CAPLUS
- (18) Takeda Chemical Industries Ltd; JP 11193281 A CAPLUS
- (19) Takeda Chemical Industries Ltd; AU 9896480 A CAPLUS
- (20) Takeda Chemical Industries Ltd; WO 9921555 A2 1999 CAPLUS

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L22 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2001:31464 CAPLUS  
DN 134:100762  
ED Entered STN: 12 Jan 2001  
TI Preparation of pyridine derivatives and medicinal use thereof  
IN Iino, Yukio; Fujita, Kohichi; Kodaira, Ariko; Hatanaka, Toshihiro;  
Takehana, Kenji; Kobayashi, Tsuyoshi; Konishi, Atsushi; Yamamoto, Takashi  
PA Ajinomoto Co., Inc., Japan  
SO PCT Int. Appl., 86 pp.  
CODEN: PIXXD2  
DT Patent  
LA Japanese  
IC C07D211-58; C07D213-75; C07D213-76; C07D237-20; C07D237-22; C07D239-42;  
C07D239-48; C07D277-44; A61K031-44; A61K031-445; A61K031-50; A61K031-505;  
A61P029-00  
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 1  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002359	A1	20010111	WO 2000-JP4298	20000629
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	EP 1193255	A1	20020403	EP 2000-940879	20000629
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
	BR 2000012046	A	20020514	BR 2000-12046	20000629
	TW 519538	B	20030201	TW 2000-89113050	20000630
	US 2002133005	A1	20020919	US 2001-29871	20011231
PRAI	JP 1999-187959	A	19990701		
	JP 2000-71706	A	20000315		
	WO 2000-JP4298	W	20000629		
OS	MARPAT 134:100762				
GI					



AB Heterocyclic compds. represented by the following general formula  
R1-CO-N(R2)-A-X-B-N(R3)-Y-(CH2)n-R4 [R1 = (un)substituted or cycloalkenyl;  
R2, R3 = H, alkyl; R4 = (un)substituted alkyl, alkenyl, cycloalkyl,  
cycloalkenyl, aryl, or heterocyclyl having .gtoreq.1 heteroatom(s); A =  
(un)substituted heterocyclic ring; B = (un)substituted arom. or  
heterocyclic ring; n = 0-6; Y = a bond between atoms, CO, CO2, CONR5,  
C(S)NR5, SO, SO2 (wherein R5 = H, alkyl); X = a bond between atoms, O,



OCHR7, CHR80, O2C, CO2, OC(S), C(S)O, S, SO, SO2, SCHR9, CHR10S, SC(O), C(O)S, SC(S), C(S)S, SO2 NR11, NR12SO2, NR13, etc.; R7 - R10 = H, alkyl; R11 - R13 = H, alkyl, acyl] or pharmacol. acceptable salts thereof are prepd. These compds. have inhibitory effects on AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor, etc. and are usable as drugs such as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics. Thus, 2-mercapto-5-nitropyridine was treated with NaH in DMF and then alkylated by 1-bromomethyl-4-nitrobenzene at room temp. for 1.5 h to give 2-(4-nitrobenzylthio)-5-nitropyridine which was reduced by Zn/AcOH in THF at room temp. for 16 h to 2-(4-aminobenzylthio)-5-aminopyridine and then acylated by 2,2-dimethylcyclopropanecarbonyl chloride in the presence of Et3N in CH2Cl2 at room temp. for 17 h to give 2-(4-(2,2-dimethylcyclopropanecarbonylamino)benzylthio)-5-(2,2-dimethylcyclopropanecarbonylamino)pyridine (I). I in vitro inhibited NF-kappa B activity with IC50 of 0.015 .mu.g/mL in an assay measuring .beta.-galactosidase activity expressed in HUVEC cells and driven by NF-kappa B-binding sequence-fused SV40 T antigen min. promoter.

ST pyridine prepn antiinflammatory; antirheumatic pyridine prepn; **antiviral** immunosuppressant pyridine prepn; cancer metastasis inhibitor pyridine prepn; antiarteriosclerotics pyridine prepn

IT Transcription factors  
 RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
 (AP-1 (activator protein 1); prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Transcription factors  
 RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
 (NF-kappa B (nuclear factor .kappa. B); prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Cell adhesion  
 (factor, inflammatory; prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Cytokines  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (inflammatory; prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Antitumor agents  
 (metastasis; prepn. of pyridine derivs. as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics)

IT Anti-inflammatory agents  
 Antiarteriosclerotics  
 Antirheumatic agents  
**Antiviral** agents  
 Immunosuppressants  
 (prepn. of pyridine derivs. as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics)

IT 318967-19-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 318967-14-5P 318967-15-6P 318967-16-7P 318967-17-8P 318967-18-9P  
 318967-20-3P 318967-21-4P 318967-22-5P 318967-23-6P 318967-24-7P  
 318967-25-8P 318967-26-9P **318967-27-0P** 318967-28-1P  
 318967-29-2P 318967-30-5P 318967-31-6P 318967-32-7P 318967-33-8P  
 318967-34-9P 318967-35-0P 318967-36-1P 318967-37-2P 318967-38-3P  
 318967-39-4P 318967-40-7P 318967-41-8P 318967-42-9P 318967-43-0P  
 318967-44-1P 318967-45-2P 318967-46-3P 318967-47-4P 318967-48-5P  
 318967-49-6P 318967-50-9P 318967-51-0P 318967-52-1P 318967-53-2P  
 318967-54-3P 318967-55-4P 318967-56-5P 318967-57-6P 318967-58-7P  
 318967-59-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 81669-70-7, Metalloprotease

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 88-75-5, 2-Nitrophenol 98-09-9, Benzenesulfonyl chloride 98-88-4, Benzoyl chloride 100-02-7, 4-Nitrophenol, reactions 100-11-8, 4-Nitrobenzyl bromide 103-63-9, 2-Bromoethylbenzene 103-71-9, Phenyl isocyanate, reactions 103-72-0, Phenyl isothiocyanate 103-80-0, Phenylacetyl chloride 104-03-0, 4-Nitrophenylacetic acid 108-24-7, Acetic anhydride 122-04-3, 4-Nitrobenzoyl chloride 123-30-8, 4-Hydroxyaniline 554-84-7, 3-Nitrophenol 636-98-6, 1-Iodo-4-nitrobenzene 637-59-2, 3-Phenylpropyl bromide 661-69-8, Hexamethylditin 932-67-2, 3-Cyclohexanecarbonyl chloride 1821-12-1, 4-Phenylbutanoic acid 1849-36-1, 4-Nitrobenzenethiol 2127-09-5, 2-Mercapto-5-nitropyridine 2581-34-2, 3-Methyl-4-nitrophenol 2719-27-9, Cyclohexanecarbonyl chloride 3073-77-6, 2-Amino-5-nitropyrimidine 3958-57-4, 3-Nitrobenzyl bromide 3958-60-9, 2-Nitrobenzyl bromide 4487-59-6, 2-Bromo-5-nitropyridine 4548-45-2, 2-Chloro-5-nitropyridine 4693-91-8, 4-Methoxyphenylacetyl chloride 5339-26-4, 2-(4-Nitrophenyl)ethyl bromide 5365-15-1, 2,2-Dichlorocyclopropanecarbonyl chloride 5418-51-9, 2-Hydroxy-5-nitropyridine 5469-69-2, 3-Amino-6-chloropyridazine 7169-97-3, 2-Acetamido-5-bromopyridine 10313-60-7, 3,4-Dimethoxyphenylacetyl chloride 14221-01-3, Tetrakis(triphenylphosphine)palladium 23056-33-9, 2-Chloro-4-methyl-5-nitropyridine 24424-99-5, Di-tert-butyl dicarbonate 25026-34-0, 4-Chlorophenylacetyl chloride 33332-29-5 39053-78-6, 3,4,5-Trimethoxyphenylacetyl chloride 50541-93-0, 4-Amino-1-benzylpiperidine 50675-57-5, 2,2-Dimethylcyclopropanecarbonyl chloride 54840-15-2, 4-(tert-Butoxycarbonylamino)phenol 55972-71-9, p-Phenylenediamine hydrochloride 60733-34-8, 2-Methylcyclopropanecarbonyl chloride 69097-20-7, Tris(trimethylsiloxy)ethylene 89312-77-6 90403-98-8, 2-Methylcyclohexanecarbonyl chloride 103554-20-7 193204-58-9 318967-66-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 4982-09-6P 13534-97-9P, 5-Amino-2-bromopyridine 24253-19-8P  
 29958-19-8P 32605-02-0P 34295-27-7P 99844-01-6P 109899-69-6P  
 116735-74-1P 318967-60-1P 318967-61-2P 318967-62-3P 318967-63-4P  
 318967-64-5P 318967-65-6P 318967-67-8P 318967-68-9P 318967-69-0P  
 318967-70-3P 318967-71-4P 318967-72-5P 318967-73-6P 318967-74-7P  
 318967-75-8P 318967-76-9P **318967-77-0P 318967-78-1P**  
 318967-79-2P 318967-80-5P 318967-81-6P 318967-82-7P 318967-83-8P  
 318967-84-9P 318967-85-0P 319459-36-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE

- (1) Ajinomoto Co Inc; WO 200015603 A1 2000
- (2) Boehringer Ingelheim Pharmaceuticals Inc; JP 2000502702 A
- (3) Boehringer Ingelheim Pharmaceuticals Inc; US 6057451 A CAPLUS
- (4) Boehringer Ingelheim Pharmaceuticals Inc; WO 9724343 A1 1997 CAPLUS
- (5) Smithkline Beecham Corp; JP 2000500464 A
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- (7) Smithkline Beecham Corp; EP 866700 A1 CAPLUS
- (8) Smithkline Beecham Corp; EP 866700 A1 CAPLUS
- (9) Smithkline Beecham Corp; WO 9717958 A1 1997 CAPLUS
- (10) Smithkline Beecham Corp; WO 9717958 A1 1997 CAPLUS

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L22 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:10451 CAPLUS

DN 136:85837

ED Entered STN: 04 Jan 2002

TI Preparation of benzodiazepines as inhibitors of HPV E1 helicase

IN Hurst, David Nigel; Jones, Philip Stephen; Parkes, Kevin Edward Burdon; Parratt, Martin John; Wilson, Francis Xavier

PA F. Hoffmann-La Roche A.-G., Switz.

SO PCT Int. Appl., 119 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D243-14

ICS C07D401-06; C07D403-06; C07D471-04; C07D401-12; C07D417-12;  
 C07D413-12; C07D403-12; C07D487-04; A61K031-5513; A61K031-5517;  
 A61K031-5517; C07D471-04; C07D243-00; C07D209-00; C07D487-04;  
 C07D243-00; C07D235-00

CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))

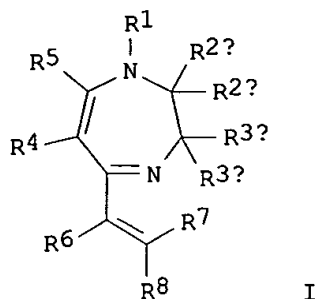
Section cross-reference(s): 1, 7

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002000632	A1	20020103	WO 2001-EP6895	20010619
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1299364	A1	20030409	EP 2001-949420	20010619

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2002128262 A1 20020912 US 2001-892148 20010626  
PRAI GB 2000-15904 A 20000628  
WO 2001-EP6895 W 20010619  
OS MARPAT 136:85837  
GI



- AB Novel benzodiazepin derivs. of general formula (I; R1 = H, lower alkyl, lower alkenyl, lower alkynyl, aryl lower alkyl, lower alkyl carbonyl, aryl carbonyl, lower alkyl aminocarbonyl, aryl aminocarbonyl, lower alkoxy carbonyl, aryloxy carbonyl; R2a, R2b = H or lower alkyl or R2a and R2b together are oxo, R1 and R2a or R2b together with the nitrogen and the carbon atom to which they are attached form an optionally substituted heterocycle; R3a, R3b = H or lower alkyl; R4 and R5 together with the two carbon atoms to which they are attached form an optionally substituted aryl or an optionally substituted heterocycle; R6, R7 = H or lower alkyl; and R8 = optionally substituted aryl or heterocyclyl) or pharmaceutically acceptable salts thereof are prepd. The novel compds. are inhibitors of the human papilloma virus (HPV) E1 helicase enzyme which is involved in the viral replication and can therefore be used as therapeutic agents for HPV mediated diseases such as visible genital warts (sexually transmitted disease) and benign external warts. Thus, a mixt. of 1.475 g (5 mmol) of (E)-3-(3,4-dichlorophenyl)-1-(2-fluorophenyl)propenone and 1.1 g (5.45 mmol) of N-[2-(isopropylamino)ethyl]pivalamide was refluxed in 10 mL of pyridine for 6 h, followed by evapn. of the solvent and silica gel chromatog. to give (26 mg E)-3-(3,4-dichlorophenyl)-1-(2-(N-(2-pivaloylaminoethyl)isopropylamino)phenyl)-2-propen-1-one as a yellow gum. The latter compd. was added a soln. of 50 mg (0.26 mmol) of 4-toluenesulfonic acid in 5 mL of acetonitrile and refluxed for 30 s, followed by evapn. of the solvent, and the residue was treated with 5 mL of methanol and 50 mg (0.5 mmol) of triethylamine and refluxed for 1 min to give, after work-up and treatment with HCl/EtOAc, (E)-5-(3,4-dichlorostyryl)-2,3-dihydro-1-isopropyl-1H-1,4-benzodiazepine dihydrochloride (II). II and (E)-5-[2-(4-Chlorophenylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride showed IC50 of .mu.g/mL against of 1.6 and 2 .mu.M, resp., against helicase.
- ST benzodiazepine prepn inhibitor HPV E1 helicase;  
styryldihydrobenzodiazepine prepn human papilloma virus E1 helicase;  
visible genital wart treatment styryldihydrobenzodiazepine prepn; benign external wart treatment styryldihydrobenzodiazepine prepn
- IT Human papillomavirus  
(E1; prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)
- IT Enzymes, biological studies  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(RNA helicase; prepn. of benzodiazepines as inhibitors of HPV E1

helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT **Antiviral agents**

Wart

(prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT 386214-96-6P, (E)-5-(3,4-Difluorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-12-9P, (E)-5-(2-Benzylthio-5-nitrostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-36-7P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-nitro-1H-1,4-benzodiazepine hydrochloride 386215-67-4P, (E)-2,3-Dihydro-1-methyl-5-[5-nitro-2-(3-phenylpropylthio)styryl]-1H-1,4-benzodiazepine 386215-85-6P 386216-22-4P, (E)-5-(3,4-Dichlorostyryl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one 386216-24-6P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-benzo-1,4-diazepine dihydrochloride 386216-30-4P 386216-48-4P 386216-58-6P 386216-68-8P 386216-74-6P 386216-75-7P 386216-86-0P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(intermediate; prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT 204130-58-5P, 2-(N-Benzyl-N-methylamino)-5-nitrobenzaldehyde 386214-97-7P, [1-Methyl-1,2,3,4-tetrahydrobenzo[e][1,4]diazepin-5-ylidenemethyl]phosphonic acid diethyl ester 386214-98-8P, [2-(2-Fluorophenyl)-2-oxoethyl]phosphonic acid diethyl ester 386215-19-6P, N-Methoxy-N-methyl-2-phenethylbenzamide 386215-25-4P 386215-41-4P 386215-46-9P 386215-48-1P 386215-51-6P 386215-89-0P 386215-99-2P 386216-04-2P 386216-06-4P 386216-09-7P 386216-16-6P, (E)-N-[[N-[2-(3-(3,4-Dichlorophenyl)acryloyl]phenyl)-N-methylcarbamoyl]methyl]pivalamide 386216-17-7P 386216-18-8P 386216-19-9P, N-[[N-(2-Acetylphenyl)-N-methylcarbamoyl]methyl]pivalamide 386216-25-7P, (E)-3-(3,4-Dichlorophenyl)-1-(2-fluorophenyl)propenone 386216-31-5P, (3-Acetyl-4-fluorophenyl)carbamic acid tert-butyl ester 386216-39-3P, N-[2-(Isopropylamino)ethyl]pivalamide 386216-40-6P, (E)-3-(3,4-Dichlorophenyl)-1-(2-(N-(2-pivaloylaminoethyl)isopropylamino)phenyl)-2-propen-1-one 386216-59-7P, Ethyl (E)-2-[5-(3,4-dichlorostyryl)-2,3-dihydro-1,4-benzodiazepin-1-yl]acetate 386216-64-4P 386216-69-9P, [2-(4-Formylbenzoylamino)ethyl]carbamic acid tert-butyl ester  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT 386216-27-9P 386216-70-2P 386216-91-7P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT 386214-99-9P, (E)-5-(4-Butoxystyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-00-5P, (E)-2,3-Dihydro-1-methyl-5-(3-phenoxytyryl)-1H-1,4-benzodiazepine dihydrochloride 386215-01-6P, (E)-5-(3-Bromo-4-methoxytyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-02-7P, (E)-5-[3-Fluoro-4-(trifluoromethyl)styryl]-2,3-dihydro-1-methyl-1H-benzo[e][1,4]diazepine dihydrochloride 386215-03-8P 386215-04-9P 386215-05-0P **386215-06-1P** 386215-07-2P 386215-08-3P 386215-09-4P 386215-10-7P 386215-11-8P, (E)-5-(2-Fluorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-13-0P, (E)-5-[2-[(2-Chloro-5-

thiazolyl)methoxy]styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine  
386215-14-1P, (E)-5-[2-(tert-Butylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-  
benzodiazepine 386215-15-2P, (E)-5-(2-Hexyloxystyryl)-2,3-dihydro-1-  
methyl-1H-1,4-benzodiazepine 386215-16-3P, (E)-2,3-Dihydro-1-methyl-5-[5-  
nitro-2-(3-pyridyloxy)styryl]-1H-1,4-benzodiazepine 386215-17-4P,  
(E)-5-(5-Bromo-2-isopropoxystyryl)-2,3-dihydro-1-methyl-1H-1,4-  
benzodiazepine 386215-18-5P, (E)-2,3-Dihydro-1-methyl-5-[2-(2-  
phenylethyl)styryl]-1H-1,4-benzodiazepine 386215-20-9P,  
(E)-2,3-Dihydro-1-methyl-5-(2-methylthiostyryl)-1H-1,4-benzodiazepine  
386215-21-0P 386215-22-1P, (E,E)-2,3-Dihydro-1-methyl-5-(2-styrylstyryl)-  
1H-1,4-benzodiazepine 386215-23-2P 386215-24-3P, (E,E)-2,3-Dihydro-1-  
methyl-5-[2-(styrylthio)styryl]-1H-1,4-benzodiazepine 386215-26-5P  
386215-27-6P, (E)-5-[2-(Cyclohexylmethylthio)styryl]-2,3-dihydro-1-methyl-  
1H-1,4-benzodiazepine 386215-28-7P, (E)-5-(3,4-Dichlorostyryl)-2,3-  
dihydro-1-methyl-1H-pyrido[2,3-e][1,4]diazepine hydrochloride  
386215-29-8P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-  
pyrido[3,4-e][1,4]diazepine 386215-30-1P, (E)-5-(3,4-Dichlorostyryl)-2,3-  
dihydro-1-methyl-1H-pyrido[3,2-e][1,4]diazepine 386215-31-2P  
386215-32-3P, (E)-5-(3,4-Dichlorostyryl)-8-(trifluoromethyl)-2,3-dihydro-1-  
methyl-1H-1,4-benzodiazepine hydrochloride 386215-33-4P,  
(E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-8-methoxy-1-methyl-1H-1,4-  
benzodiazepine hydrochloride 386215-34-5P 386215-35-6P,  
(E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-7-nitro-1H-1,4-  
benzodiazepine 386215-37-8P, (E)-5-(3,4-Dichlorostyryl)-9-  
(trifluoromethyl)-2,3-dihydro-1H-1,4-benzodiazepine dihydrochloride  
386215-38-9P, (E)-5-(3,4-Dichlorostyryl)-8-(trifluoromethyl)-2,3-dihydro-  
1H-1,4-benzodiazepine hydrochloride 386215-39-0P 386215-40-3P,  
(E)-8-Bromo-5-(3,4-dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-  
benzodiazepine dihydrochloride 386215-42-5P 386215-43-6P,  
(E)-5-(2-Benzylthio-5-nitrostyryl)-8-bromo-2,3-dihydro-1-methyl-1H-1,4-  
benzodiazepine dihydrochloride **386215-44-7P** 386215-45-8P,  
(E)-9-Chloro-5-(3,4-dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine  
dihydrochloride 386215-47-0P 386215-49-2P, (E)-5-(2-Benzylthio-5-  
nitrostyryl)-7-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine  
dihydrochloride 386215-50-5P, (E)-8-Chloro-5-(3,4-dichlorostyryl)-2,3-  
dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-52-7P  
386215-53-8P, (E)-5-(3-Allyloxystyryl)-8-chloro-2,3-dihydro-1-methyl-1H-  
1,4-benzodiazepine dihydrochloride 386215-54-9P, (E)-5-(3-  
Benzyloxystyryl)-8-chloro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine  
dihydrochloride 386215-55-0P, (E)-5-(2-Benzylthiostyryl)-2,3-dihydro-1-  
methyl-1H-1,4-benzodiazepine dihydrochloride 386215-56-1P  
386215-57-2P, (E)-5-[2-(4-Chlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-  
1,4-benzodiazepine dihydrochloride 386215-58-3P, (E)-5-[2-(3,4-  
Dichlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine  
dihydrochloride 386215-59-4P, 5-[3-Chloro-2-(4-chlorobenzylthio)styryl]-  
2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-60-7P,  
(E)-2,3-Dihydro-1-methyl-5-(5-nitro-2-phenoxy)styryl]-1H-1,4-benzodiazepine  
dihydrochloride 386215-61-8P, (E)-2,3-Dihydro-1-methyl-5-[2-(4-  
methylbenzylthio)styryl]-1H-1,4-benzodiazepine dihydrochloride  
386215-62-9P, (E)-2,3-Dihydro-5-[2-(4-methoxybenzylthio)styryl]-1-methyl-  
1H-1,4-benzodiazepine dihydrochloride 386215-63-0P, (E)-5-[2-(4-  
Chlorophenoxy)-5-nitrostyryl]-3,4-dihydro-1-methyl-1H-1,4-benzodiazepine  
hydrochloride 386215-64-1P, (E)-5-[2-(4-tert-Butylbenzylthio)styryl]-2,3-  
dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-65-2P,  
(E)-5-[2-[3-(Trifluoromethyl)benzylthio]styryl]-2,3-dihydro-1-methyl-1H-  
1,4-benzodiazepine dihydrochloride 386215-66-3P, (E)-5-[4-Bromo-2-(4-  
chlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine  
dihydrochloride 386215-68-5P, (E)-2,3-Dihydro-1-methyl-5-(2-  
pentylthiostyryl)-1H-1,4-benzodiazepine 386215-69-6P,  
(E)-5-[2-Chloro-6-(4-chlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-  
benzodiazepine hydrochloride 386215-70-9P, 2-[2-(2,3-Dihydro-1-methyl-1H-  
1,4-benzodiazepin-5-yl)vinyl]-N-methyl-4-nitroaniline dihydrochloride

386215-71-0P 386215-72-1P, (E)-5-[2-(4-Chlorophenoxy)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-73-2P, (E)-2,3-Dihydro-1-methyl-5-[2-(2-naphthylthio)styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-74-3P, (E)-2,3-Dihydro-1-methyl-5-[2-(1-naphthylthio)styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-75-4P, (E)-2,3-Dihydro-1-methyl-5-(2-p-tolylthio)styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-76-5P, (E)-2,3-Dihydro-5-[2-(4-methoxyphenylthio)styryl]-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-77-6P, (E)-2,3-Dihydro-1-methyl-5-[2-(2-naphthylthio)styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-78-7P, (E)-2,3-Dihydro-1-methyl-5-[2-[(2-naphthyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-79-8P, (E)-5-[2-[4-(Trifluoromethyl)benzyloxy]styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-80-1P, (E)-2,3-Dihydro-1-methyl-5-[2-(4-nitrobenzyloxy)styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-81-2P, (E)-5-[2-(3,4-Difluorobenzyloxy)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-82-3P, (E)-5-(2-Benzyloxystyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-83-4P, (E)-5-[2-(4-Chlorobenzyloxy)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-84-5P 386215-86-7P 386215-87-8P 386215-88-9P, (E)-2,3-Dihydro-1-methyl-5-[3-[(2-pyridyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-90-3P, (E)-2,3-Dihydro-1-methyl-5-[3-[(3-pyridyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-91-4P, (E)-2,3-Dihydro-1-methyl-5-[3-[(4-pyridyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-92-5P, (E)-2,3-Dihydro-1-methyl-5-[3-[(5-methyl-3-isoxazolyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-93-6P, (E)-5-[3-[(1-Benzyl-1H-imidazol-2-yl)methoxy]styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-94-7P, (E)-5-[2,3-Dihydro-3-(4-methoxybenzyloxy)styryl]-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-95-8P 386215-96-9P, (E)-2,3-Dihydro-1-methyl-5-[3-[(3,5-dimethyl-1-pyrazolyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-97-0P 386215-98-1P, (E)-5-[2-(4-Chlorophenoxy)styryl]-8-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-00-8P, (E)-5-[3-Chloro-2-(3,4-dichlorobenzylthio)styryl]-8-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-01-9P, (E)-5-(2-Benzylthio)styryl)-8-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-02-0P, (E)-5-(2-Benzylthio-5-nitrostyryl)-8-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-03-1P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-8-(3-methoxyphenyl)-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-05-3P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-phenyl-1H-1,4-benzodiazepine dihydrochloride 386216-07-5P 386216-08-6P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-(3-thienyl)-1H-1,4-benzodiazepine dihydrochloride 386216-10-0P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-9-phenyl-1H-1,4-benzodiazepine dihydrochloride 386216-11-1P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-9-(4-methoxyphenyl)-1H-1,4-benzodiazepine dihydrochloride 386216-12-2P, (E)-5-[2-(4-Chlorophenylthio)styryl]-2,3-dihydro-1-methyl-8-(3-thienyl)-1H-1,4-benzodiazepine dihydrochloride 386216-13-3P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-vinyl-1H-1,4-benzodiazepine dihydrochloride 386216-14-4P, (E)-5-[2-(4-Chlorophenylthio)styryl]-8-(2-furyl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-15-5P, (E)-5-(3,4-Dichlorostyryl)-1,3-dihydro-1-methyl-2H-benzo-1,4-diazepin-2-one 386216-20-2P, (E)-1,3-Dihydro-5-styryl-2H-benzo-1,4-diazepin-2-one 386216-21-3P, (E)-5-(2,3-Dichlorostyryl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one 386216-23-5P, (E)-5-[2-(4-Chlorophenylthio)styryl]-2,3-dihydro-1H-1,4-benzodiazepine dihydrochloride 386216-26-8P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-benzo-1,4-diazepine dihydrochloride 386216-29-1P 386216-32-6P, (E)-5-(3,4-Dichlorostyryl)-1-ethyl-2,3-dihydro-1H-1,4-benzodiazepine dihydrochloride 386216-33-7P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-

propyl-1H-1,4-benzodiazepine dihydrochloride 386216-34-8P,  
 (E)-1-Benzyl-5-(3,4-dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine  
 dihydrochloride 386216-35-9P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-  
 1,4-benzodiazepine-1-ethanol dihydrochloride 386216-36-0P,  
 (E)-5-[2-(4-Chlorophenylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-  
 benzodiazepine dihydrochloride 386216-37-1P 386216-38-2P,  
 (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-isopropyl-1H-1,4-benzodiazepine  
 dihydrochloride 386216-41-7P, (E)-1-Acetyl-5-(3,4-dichlorostyryl)-2,3-  
 dihydro-1H-1,4-benzodiazepine hydrochloride 386216-43-9P,  
 (E)-1-Benzoyl-5-(3,4-dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine  
 hydrochloride 386216-44-0P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-(4-  
 nitrobenzyl)-1H-1,4-benzodiazepine dihydrochloride 386216-45-1P  
 386216-46-2P 386216-47-3P 386216-49-5P, (E)-5-(3,4-Dichlorostyryl)-2,3-  
 dihydro-1-[(2-naphthyl)methyl]-1H-1,4-benzodiazepine dihydrochloride  
 386216-50-8P, (E)-4-[[5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-1,4-  
 benzodiazepin-1-yl]methyl]benzoic acid dihydrochloride 386216-52-0P,  
 (E)-3-[[5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepin-1-  
 yl]methyl]benzoic acid hydrochloride 386216-54-2P, (E)-2-[[5-(3,4-  
 Dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepin-1-yl]methyl]benzoic acid  
 hydrochloride 386216-56-4P, (E)-4-[[5-(2-(4-Chlorophenylthio)styryl)-2,3-  
 dihydro-1H-1,4-benzodiazepin-1-yl]methyl]benzoic acid hydrochloride  
 386216-57-5P, (E)-5-(3,4-Dichlorostyryl)-N-ethyl-2,3-dihydro-1H-1,4-  
 benzodiazepine-1-carboxamide 386216-60-0P, (E)-5-(3,4-Dichlorostyryl)-  
 2,3-dihydro-N-(2-methoxyethyl)-1H-1,4-benzodiazepine-1-acetamide  
 dihydrochloride 386216-61-1P 386216-63-3P 386216-65-5P  
 386216-66-6P 386216-67-7P 386216-71-3P 386216-72-4P 386216-73-5P  
 386216-76-8P 386216-77-9P 386216-78-0P 386216-79-1P 386216-80-4P  
 386216-81-5P, 4-[2-(2,3-Dihydro-1-methyl-1H-1,4-benzodiazepin-5-  
 yl)vinyl]benzamide hydrochloride 386216-82-6P, (E)-5-(3,4-  
 Dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepin-8-ol  
 hydrochloride 386216-83-7P 386216-85-9P 386216-87-1P,  
 (E)-N-[5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepin-7-  
 yl]methanesulfonamide 386216-88-2P, (E)-5-(3,4-Dichlorostyryl)-2,3-  
 dihydro-8-(4-methoxyphenyl)-1-methyl-1H-1,4-benzodiazepine 386216-89-3P,  
 (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-(2-thienyl)-1H-1,4-  
 benzodiazepine hydrochloride 386216-90-6P, (E)-5-(3,4-Dichlorostyryl)-  
 2,3-dihydro-1-methyl-1H-1,4-benzodiazepin-8-amine hydrochloride  
 386216-93-9P 386216-94-0P 386216-95-1P 386216-97-3P,  
 (E)-2,3-Dihydro-5-(4-methoxystyryl)-1-methyl-1H-1,4-benzodiazepine  
 hydrochloride 386216-98-4P, (E)-2,3-Dihydro-1-methyl-5-(4-phenoxytyryl)-  
 1H-1,4-benzodiazepine hydrochloride 386216-99-5P, (E)-2,3-Dihydro-1-  
 methyl-5-styryl-1H-1,4-benzodiazepine dihydrochloride 386217-00-1P,  
 (E)-5-(3,4-Dichlorostyryl)-1,3-dihydro-7,8-dimethoxy-2H-1,4-benzodiazepin-  
 2-one 386217-01-2P, (E)-1-Acetyl-5-(3,4-dichlorostyryl)-2,3-dihydro-1H-  
 1,4-benzodiazepine dihydrochloride 386217-02-3P, (E)-5-(3,4-  
 Dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine-1-ethanol hydrochloride  
 386217-03-4P 386217-04-5P, 5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-  
 vinyl-1H-1,4-benzodiazepine dihydrochloride 386217-05-6P 386217-06-7P  
 386217-07-8P 386217-08-9P 386217-09-0P 386217-10-3P,  
 (E)-5-[3-Chloro-2-(4-chlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-  
 benzodiazepine dihydrochloride 386217-11-4P 386224-42-6P,  
 (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepin-7-  
 acetamide hydrochloride

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(prepn. of benzodiazepines as inhibitors of HPV E1 helicase and  
 therapeutic agents for HPV mediated diseases such as visible genital  
 warts and benign external warts)

IT 67-36-7, 4-Phenoxybenzaldehyde 90-02-8, 2-Hydroxybenzaldehyde, reactions  
 93-97-0, Benzoic anhydride 98-80-6, Phenylboronic acid 100-11-8,  
 4-Nitrobenzyl bromide 100-52-7, Benzaldehyde, reactions 100-53-8,



Benzylmercaptan 103-67-3, N-Benzylmethylamine 105-36-2, Ethyl  
 bromoacetate 106-48-9, 4-Chlorophenol 107-15-3, Ethylenediamine,  
 reactions 109-81-9, N-Methylethylenediamine 109-85-3,  
 2-Methoxyethylamine 109-90-0, Ethyl isocyanate 110-72-5,  
 N-Ethylethylenediamine 111-39-7, N-Propylethylenediamine 111-41-1,  
 2-(2-Aminoethylamino)ethanol 123-11-5, 4-Methoxybenzaldehyde, reactions  
 147-93-3, Thiosalicylic acid 445-29-4, 2-Fluorobenzoic acid 446-30-0,  
 4-Chloro-2-fluorobenzoic acid 446-52-6, 2-Fluorobenzaldehyde 450-95-3,  
 2-Fluoroacetophenone 543-24-8, N-Acetylglycine 551-93-9,  
 2'-Aminoacetophenone 586-98-1, 2-Pyridylmethanol 598-21-0, Bromoacetyl  
 bromide 619-66-9, 4-Carboxybenzaldehyde 636-72-6, Thiophene-2-methanol  
 939-26-4, 2-Bromomethylnaphthalene 1126-81-4, 4-Acetamidothiophenol  
 1129-28-8, Methyl 3-(bromomethyl)benzoate 1571-08-0, Methyl  
 4-formylbenzoate 1583-58-0, 2,4-Difluorobenzoic acid 1859-75-2,  
 2'-(Methylamino)acetophenone 2393-23-9, 4-Methoxybenzylamine  
 2417-72-3, Methyl 4-(bromomethyl)benzoate 2417-73-4, Methyl  
 2-(bromomethyl)benzoate 2991-28-8, 2,5-Difluorobenzoic acid 2999-46-4,  
 Ethyl isocyanoacetate 3006-96-0, 4-Hydroxymethylbenzoic acid  
 3095-95-2, Diethylphosphonoacetic acid 4152-09-4, N-  
 Benzylethylenediamine 4392-24-9, Cinnamyl bromide 4890-85-1,  
 2-Phenethylbenzoic acid 5071-96-5, 3-Methoxybenzylamine 5720-07-0,  
 4-Methoxyphenylboronic acid 6165-68-0, Thiophene-2-boronic acid  
 6165-69-1, Thiophene-3-boronic acid 6258-66-8, 4-Chlorobenzylmercaptan  
 6287-38-3, 3,4-Dichlorobenzaldehyde 6334-18-5, 2,3-Dichlorobenzaldehyde  
 6361-21-3, 2-Chloro-5-nitrobenzaldehyde 6361-22-4, 2-Chloro-6-  
 nitrobenzaldehyde 6850-57-3, 2-Methoxybenzylamine 7486-35-3,  
 Vinyltributylstannane 10365-98-7, 3-Methoxyphenylboronic acid  
 19522-67-9, N-Isopropylethylenediamine 24424-99-5, Di-tert-butyl  
 dicarbonate 32832-96-5, 2-Phenethylbenzaldehyde 34036-07-2,  
 3,4-Difluorobenzaldehyde 36480-40-7, 3,4-Dichlorobenzyl mercaptan  
 57260-73-8, N-(2-Aminoethyl)carbamic acid tert-butyl ester 67500-19-0,  
 1-(5-Amino-2-fluorophenyl)ethanone 85070-48-0, 3-Chloro-2-  
 fluorobenzaldehyde 107572-07-6, 2-(4-Chlorophenylthio)benzaldehyde  
 112704-79-7, 2-Fluoro-4-bromobenzoic acid 118486-94-5,  
 2-(Tributylstannyl)furan 142265-69-8, 1-(2-Fluoro-4,5-  
 dimethoxyphenyl)ethanone 161957-55-7, 2-Fluoro-3-chlorobenzoic acid  
 174013-29-7, 2-Fluoro-6-trifluoromethylacetophenone 175278-43-0,  
 2-Benzylthio-5-nitrobenzaldehyde 376646-64-9, 3-Formyl-4-(3-  
 bromophenyl)pyridine 386216-28-0 386216-42-8, (E)-5-(3,4-  
 Dichlorostyryl)-2,3-dihydro-1H-benzo-1,4-diazepine 386216-51-9  
 386216-53-1 386216-55-3 386216-92-8, 4-(3-Bromophenyl)-2-  
 formylpyridine 386216-96-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; prepn. of benzodiazepines as inhibitors of HPV E1 helicase  
 and therapeutic agents for HPV mediated diseases such as visible  
 genital warts and benign external warts)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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- (2) Duphar Int Res; EP 0350131 A 1990 CAPLUS
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- (4) La Roche, H; EP 0462522 A 1991 CAPLUS
- (5) Schmitt, J; US 3426014 A 1969

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AN 2002:256041 CAPLUS

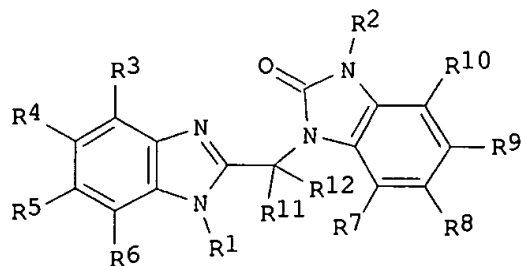
DN 136:294826

ED Entered STN: 05 Apr 2002

TI Preparation of benzimidazolone **antiviral** agents

IN Yu, Kuo-Long; Civiello, Rita; Combrink, Keith; Gulgeze, Hatice Belgin;  
 Pearce, Bradley C.; Wang, Xiangdong; Meanwell, Nicholas A.; Zhang, Yi  
 PA Bristol-Myers Squibb Company, USA  
 SO PCT Int. Appl., 216 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM A61K031-4184  
 ICS A61K031-443; A61K031-422; A61K031-427; A61K031-454; A61K031-501;  
 A61K031-5377; C07D401-14; C07D403-06; C07D403-14; C07D413-14;  
 C07D417-14  
 CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 10  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002026228	A1	20020404	WO 2001-US29493	20010927
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 6506738	B1	20030114	US 2001-952736	20010914
PRAI	US 2000-235804P	P	20000927		
OS	MARPAT 136:294826				
GI					



I

AB The title compds. [I; R1 = (CRvRw)nX; Rv, Rw = H, (halo)alkyl, (halo)alkenyl; X = H, (un)substituted alkyl, alkenyl; n = 1-6; R2 = H, alkyl, Ph, etc.; R3, R6, R7, R10 = H; R5, R8, R9 = H, halo, CF3; R4 = H, halo, CN, etc.; R11, R12 = H], useful in the treatment of viral infections, more particularly, for the treatment of respiratory syncytial virus infection, were prepd. E.g., a 4-step synthesis of I [R1 = CH2CH2CHMe2; R2 = C(:CH2)Me; R3-R12 = H], starting with 2-(chloromethyl)benzimidazole, was given. The title compds. I showed **antiviral** activity against RSV with EC50's between 50 .mu.M and 0.001 .mu.M.

ST benzimidazolone prepn **antiviral** respiratory syncytial virus RSV  
 IT **Antiviral** agents  
 (prepn. of benzimidazolone **antiviral** agents)  
 IT Respiratory syncytial virus  
 (treatment of RSV infection; prepn. of benzimidazolone **antiviral** agents)  
 IT 406940-52-1P 406940-54-3P 406940-55-4P 406940-56-5P 406940-57-6P  
 406940-63-4P 406940-76-9P 406941-33-1P 406941-36-4P 406941-69-3P

406941-70-6P	406941-71-7P	406941-78-4P	406941-83-1P	406941-84-2P
406941-87-5P	406941-89-7P	406941-92-2P	406941-93-3P	406942-22-1P
406942-26-5P	406942-39-0P	406942-55-0P	406942-56-1P	406942-59-4P
406942-60-7P	406942-63-0P	406942-68-5P	406942-72-1P	406942-82-3P
406942-84-5P	406942-86-7P	406942-87-8P	406943-03-1P	406943-05-3P
406943-11-1P	406943-18-8P	406943-20-2P	406943-22-4P	406943-25-7P
406943-29-1P	406943-53-1P	406943-55-3P	406943-56-4P	406943-68-8P
406943-71-3P	406943-84-8P	406943-85-9P	406943-86-0P	406943-89-3P
406943-97-3P	406944-07-8P	406944-12-5P	406944-22-7P	406944-23-8P
406944-36-3P	406944-45-4P	406944-48-7P	406944-59-0P	406944-76-1P
406945-21-9P				

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

	(prepn. of benzimidazolone	antiviral agents)		
IT 406940-53-2P	406940-58-7P	406940-59-8P	406940-60-1P	406940-61-2P
406940-62-3P	406940-64-5P	406940-65-6P	406940-66-7P	406940-68-9P
406940-69-0P	406940-71-4P	406940-73-6P	406940-75-8P	406940-77-0P
406940-78-1P	406940-79-2P	406940-81-6P	406940-82-7P	406940-83-8P
406940-84-9P	406940-85-0P	406940-86-1P	406940-87-2P	406940-88-3P
406940-89-4P	406940-90-7P	406940-91-8P	406940-92-9P	406940-93-0P
406940-94-1P	406940-95-2P	406940-96-3P	406940-97-4P	406940-98-5P
406940-99-6P	406941-00-2P	406941-01-3P	406941-02-4P	406941-03-5P
406941-04-6P	406941-05-7P	406941-06-8P	406941-07-9P	406941-08-0P
406941-09-1P	406941-10-4P	406941-11-5P	406941-12-6P	406941-13-7P
406941-14-8P	406941-15-9P	406941-16-0P	406941-17-1P	406941-18-2P
406941-19-3P	406941-20-6P	406941-21-7P	406941-22-8P	406941-23-9P
406941-24-0P	406941-25-1P	406941-26-2P	406941-27-3P	406941-28-4P
406941-29-5P	406941-30-8P	406941-31-9P	406941-32-0P	406941-34-2P
406941-35-3P	406941-37-5P	406941-38-6P	406941-40-0P	406941-42-2P
406941-44-4P	406941-46-6P	406941-48-8P	406941-51-3P	406941-53-5P
406941-54-6P	406941-55-7P	406941-56-8P	406941-57-9P	406941-58-0P
406941-59-1P	406941-60-4P	406941-61-5P	<b>406941-62-6P</b>	
406941-63-7P	406941-64-8P	406941-65-9P	406941-66-0P	406941-67-1P
406941-68-2P	406941-72-8P	406941-73-9P	406941-74-0P	406941-75-1P
406941-76-2P	406941-77-3P	406941-79-5P	406941-80-8P	406941-81-9P
406941-82-0P	406941-85-3P	406941-86-4P	406941-88-6P	406941-90-0P
406941-91-1P	406941-94-4P	406941-95-5P	406941-96-6P	406941-97-7P
406941-98-8P	406941-99-9P	406942-00-5P	406942-02-7P	406942-03-8P
406942-04-9P	406942-05-0P	406942-06-1P	406942-07-2P	406942-08-3P
406942-09-4P	406942-10-7P	406942-11-8P	406942-12-9P	406942-13-0P
406942-14-1P	406942-15-2P	406942-16-3P	406942-17-4P	406942-18-5P
406942-19-6P	406942-20-9P	406942-21-0P	406942-23-2P	406942-24-3P
406942-25-4P	406942-27-6P	406942-28-7P	406942-29-8P	406942-30-1P
406942-31-2P	406942-32-3P	406942-33-4P	406942-34-5P	406942-35-6P
406942-37-8P	406942-38-9P	406942-40-3P	406942-41-4P	406942-42-5P
406942-43-6P	406942-44-7P	406942-45-8P	406942-46-9P	406942-47-0P
406942-48-1P	406942-49-2P	406942-50-5P	406942-51-6P	406942-52-7P
406942-53-8P	406942-54-9P	406942-57-2P	406942-58-3P	406942-61-8P
406942-62-9P	406942-64-1P	406942-65-2P	406942-66-3P	406942-67-4P
406942-69-6P	406942-70-9P	406942-71-0P	406942-73-2P	406942-74-3P
406942-75-4P	406942-76-5P	406942-77-6P	406942-78-7P	406942-79-8P
406942-80-1P	406942-81-2P	406942-83-4P	406942-85-6P	406942-88-9P
406942-89-0P	406942-90-3P	406942-91-4P	406942-92-5P	406942-93-6P
406942-94-7P	406942-95-8P	406942-96-9P	406942-97-0P	406942-98-1P
406942-99-2P	406943-01-9P	406943-07-5P	406943-09-7P	406943-13-3P
406943-15-5P	406943-16-6P	406943-17-7P	406943-19-9P	406943-21-3P
406943-23-5P	406943-24-6P	406943-26-8P	406943-27-9P	406943-28-0P
406943-30-4P	406943-31-5P	406943-32-6P	406943-34-8P	406943-35-9P
406943-36-0P	406943-38-2P	406943-39-3P	406943-40-6P	406943-41-7P
406943-42-8P	406943-43-9P	406943-44-0P	406943-45-1P	406943-46-2P
406943-47-3P	406943-48-4P	406943-49-5P	406943-50-8P	406943-51-9P

406943-52-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolone **antiviral agents**)

IT	406943-54-2P	406943-57-5P	406943-58-6P	406943-59-7P	406943-60-0P
	406943-61-1P	406943-62-2P	406943-63-3P	406943-64-4P	406943-65-5P
	406943-66-6P	406943-67-7P	406943-69-9P	406943-70-2P	406943-72-4P
	406943-73-5P	406943-74-6P	406943-75-7P	406943-76-8P	406943-77-9P
	406943-78-0P	406943-79-1P	406943-80-4P	406943-81-5P	406943-82-6P
	406943-83-7P	406943-88-2P	406943-90-6P	406943-92-8P	406943-93-9P
	406943-94-0P	406943-95-1P	406943-96-2P	406943-98-4P	406943-99-5P
	406944-00-1P	406944-01-2P	406944-02-3P	406944-03-4P	406944-04-5P
	406944-05-6P	406944-06-7P	406944-08-9P	406944-09-0P	406944-10-3P
	406944-11-4P	406944-13-6P	406944-14-7P	406944-15-8P	406944-16-9P
	406944-17-0P	406944-18-1P	406944-19-2P	406944-20-5P	406944-21-6P
	406944-24-9P	406944-25-0P	406944-26-1P	406944-27-2P	406944-28-3P
	406944-29-4P	406944-30-7P	406944-32-9P	406944-33-0P	406944-34-1P
	406944-35-2P	406944-37-4P	406944-38-5P	406944-39-6P	406944-40-9P
	406944-41-0P	406944-42-1P	406944-43-2P	406944-44-3P	406944-46-5P
	406944-47-6P	406944-49-8P	406944-51-2P	406944-53-4P	406944-55-6P
	406944-56-7P	406944-57-8P	406944-58-9P	406944-60-3P	406944-61-4P
	406944-62-5P	406944-63-6P	406944-64-7P	406944-65-8P	406944-66-9P
	406944-67-0P	406944-68-1P	406944-69-2P	406944-70-5P	406944-71-6P
	406944-72-7P	406944-73-8P	406944-74-9P	406944-75-0P	406944-77-2P
	406944-78-3P	406944-80-7P	406944-81-8P	406944-82-9P	

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolone **antiviral agents**)

IT	60-24-2, Mercaptoethanol	66-22-8, Uracil, reactions	70-11-1, 2-Bromoacetophenone	78-94-4, Methyl vinyl ketone, reactions	79-44-7, n,N-Dimethylcarbamoyl chloride	96-32-2, Methyl bromoacetate	98-09-9, Benzenesulfonyl chloride	105-36-2, Ethyl bromoacetate	107-13-1, Acrylonitrile, reactions	107-82-4, 1-Bromo-3-methylbutane	107-85-7, 3-Methylbutylamine	108-00-9, N,N-Dimethylethylenediamine	109-01-3, N-Methylpiperazine	109-83-1, N-Methylaminoethanol	109-85-3, 2-Methoxyethylamine	109-90-0, Ethyl isocyanate	141-97-9, Ethyl acetoacetate	156-87-6, 288-13-1, Pyrazole	364-74-9, 2,5-Difluoronitrobenzene	462-72-6, 1-Bromo-4-fluorobutane	535-11-5, Ethyl 2-bromopropionate	542-81-4, 623-24-5, .alpha.,.alpha.'-Dibromo-p-xylene	626-67-5, N-Methylpiperidine	682-30-4, 683-60-3, Sodium isopropoxide	836-42-0, 4-Benzyloxybenzyl chloride	870-63-3, 1-Bromo-3-methyl-2-butene	939-80-0, 4-Chloro-3-nitrobenzonitrile	1072-52-2, 2-(Aziridin-1-yl)ethanol	1120-71-4, [1,2]Oxathiolane	2,2-dioxide	1129-28-8, Methyl 3-(bromomethyl)benzoate	1493-27-2, 2-Fluoronitrobenzene	1632-83-3, N-Methylbenzimidazole	1703-46-4, 4-(N,N-Dimethylamino)benzyl alcohol	1849-01-0, 1-Methyl-2-benzimidazolone	2417-72-3, Methyl 4-(bromomethyl)benzoate	2417-73-4, Methyl 2-(bromomethyl)benzoate	3680-02-2, Methyl vinyl sulfone	4104-45-4, 3-(Methylthio)propylamine	4584-46-7, N-(2-Chloroethyl)dimethylamine hydrochloride	4753-59-7, 4-Bromobutyl acetate	4856-97-7, 2-(Hydroxymethyl)benzimidazole	4857-04-9, 2-(Chloromethyl)benzimidazole	5292-43-3, tert-Butyl bromoacetate	5332-06-9, 4-Bromobutyronitrile	5407-04-5, N-(3-Chloropropyl)dimethylamine hydrochloride	5414-21-1, 5-Bromovaleronitrile	5465-65-6, 5978-08-5, 6232-88-8, 4-Bromomethylbenzoic acid	7250-67-1, N-(2-Chloroethyl)pyrrolidine hydrochloride	10045-45-1, 1-Ethyl-1,3-dihydrobenzimidazol-2-one	10147-37-2, Isopropylsulfonyl chloride	13220-33-2, 1-Methyl-3-hydroxypyrrolidine	13325-10-5, 1-Amino-4-butanol	13795-73-8, Di-tert-butyl aspartate	14813-85-5, 18645-88-0, 3-Fluorobenzene-1,2-diamine	19810-31-2, Benzyloxyacetyl
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chloride 20662-53-7 20780-53-4 27988-97-2, Tetrazole 32213-95-9,  
Dimethyl L-aspartate hydrochloride 32754-99-7, 4-Aminobutyronitrile  
40517-43-9, 1-(Methanesulfonyl)-4-(chloromethyl)benzene 41120-23-4  
52099-72-6, 1-Isopropenyl-2-benzimidazolone 57683-71-3,  
2-Carbomethoxybenzenesulfonamide 76179-40-3, 2-Amino-4,5-difluoroaniline  
142649-86-3 144655-76-5 161468-47-9 161468-55-9 222978-03-2,  
2-Fluoro-4-(bromomethyl)benzonitrile 406945-20-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of benzimidazolone **antiviral** agents)

IT 4113-97-7P 4926-55-0P 23937-68-0P 25238-55-5P 35562-81-3P  
35681-40-4P 43215-12-9P 51138-16-0P 56436-25-0P 56636-93-2P  
56636-95-4P 64266-27-9P 69449-20-3P 78156-03-3P 87120-81-8P  
104189-83-5P 125460-21-1P 256366-08-2P 257869-92-4P 346694-26-6P  
347355-52-6P 380543-66-8P 380604-60-4P 380604-61-5P 380604-62-6P  
380604-63-7P 380604-64-8P 380604-65-9P 380604-66-0P 380604-67-1P  
380604-70-6P 380604-71-7P 380604-72-8P 380604-73-9P 380604-83-1P  
380604-84-2P 380605-11-8P 406944-83-0P 406944-84-1P 406944-85-2P  
406944-86-3P 406944-87-4P 406944-88-5P 406944-89-6P 406944-90-9P  
406944-91-0P 406944-92-1P 406944-93-2P 406944-94-3P 406944-95-4P  
406944-96-5P 406944-97-6P 406944-98-7P 406944-99-8P 406945-00-4P  
406945-01-5P 406945-02-6P 406945-03-7P 406945-04-8P 406945-05-9P  
406945-06-0P 406945-10-6P 406945-11-7P 406945-12-8P 406945-13-9P  
406945-14-0P 406945-15-1P 406945-16-2P 406945-17-3P 406945-18-4P  
406945-19-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(prepn. of benzimidazolone **antiviral** agents)

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Meanwell; J Org Chem 1995, V60(6), P1565 CAPLUS

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	57.23	436.71
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-5.54	-11.77

FILE 'CAPLUS' ENTERED AT 10:05:00 ON 21 JAN 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4

FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004

L1 STRUCTURE UPLOADED  
L2 0 S L1 EXA SAM  
L3 0 S L1 FAM SAM  
L4 50 S L1 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004

L5 10 S L4

FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004

L6 4073 S L1 SSS FULL  
L7 3719 S HIV OR RETROVIRAL OR RETROVIRUS  
L8 2422 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004

L9 70667 S HIV OR RETROVIRAL OR RETROVIRUS  
L10 31317 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV  
L11 636 S L6  
L12 9 S L11 AND L9

FILE 'REGISTRY' ENTERED AT 09:41:14 ON 21 JAN 2004

L13 1 S 188839-16-9/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:42:34 ON 21 JAN 2004

FILE 'REGISTRY' ENTERED AT 09:47:14 ON 21 JAN 2004

L14 1 S 457949-18-7/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:48:05 ON 21 JAN 2004

L15 5 S L11 AND L10  
L16 2 S L15 NOT L12

FILE 'REGISTRY' ENTERED AT 09:49:33 ON 21 JAN 2004

L17 1 S 174398-05-1/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:50:25 ON 21 JAN 2004

FILE 'REGISTRY' ENTERED AT 09:51:38 ON 21 JAN 2004

L18 1 S 26148-35-6/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:54:26 ON 21 JAN 2004

E ANTIVIRAL  
L19 41468 S E3-E9  
L20 21 S L19 AND L11  
L21 15 S L20 NOT L12  
L22 13 S L21 NOT L16

FILE 'CAPLUS' ENTERED AT 10:05:00 ON 21 JAN 2004

=> d his

(FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004

L1 STRUCTURE UPLOADED  
L2 0 S L1 EXA SAM  
L3 0 S L1 FAM SAM  
L4 50 S L1 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004

L5 10 S L4

FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004

L6 4073 S L1 SSS FULL  
L7 3719 S HIV OR RETROVIRAL OR RETROVIRUS  
L8 2422 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004

L9 70667 S HIV OR RETROVIRAL OR RETROVIRUS  
L10 31317 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV  
L11 636 S L6  
L12 9 S L11 AND L9

FILE 'REGISTRY' ENTERED AT 09:41:14 ON 21 JAN 2004

L13 1 S 188839-16-9/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:42:34 ON 21 JAN 2004

FILE 'REGISTRY' ENTERED AT 09:47:14 ON 21 JAN 2004

L14 1 S 457949-18-7/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:48:05 ON 21 JAN 2004

L15 5 S L11 AND L10  
L16 2 S L15 NOT L12

FILE 'REGISTRY' ENTERED AT 09:49:33 ON 21 JAN 2004

L17 1 S 174398-05-1/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:50:25 ON 21 JAN 2004

FILE 'REGISTRY' ENTERED AT 09:51:38 ON 21 JAN 2004

L18 1 S 26148-35-6/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 09:54:26 ON 21 JAN 2004

E ANTIVIRAL  
L19 41468 S E3-E9  
L20 21 S L19 AND L11  
L21 15 S L20 NOT L12

L22            13 S L21 NOT L16

FILE 'CAPLUS' ENTERED AT 10:05:00 ON 21 JAN 2004

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.01	443.72
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-11.77

STN INTERNATIONAL LOGOFF AT 10:14:26 ON 21 JAN 2004